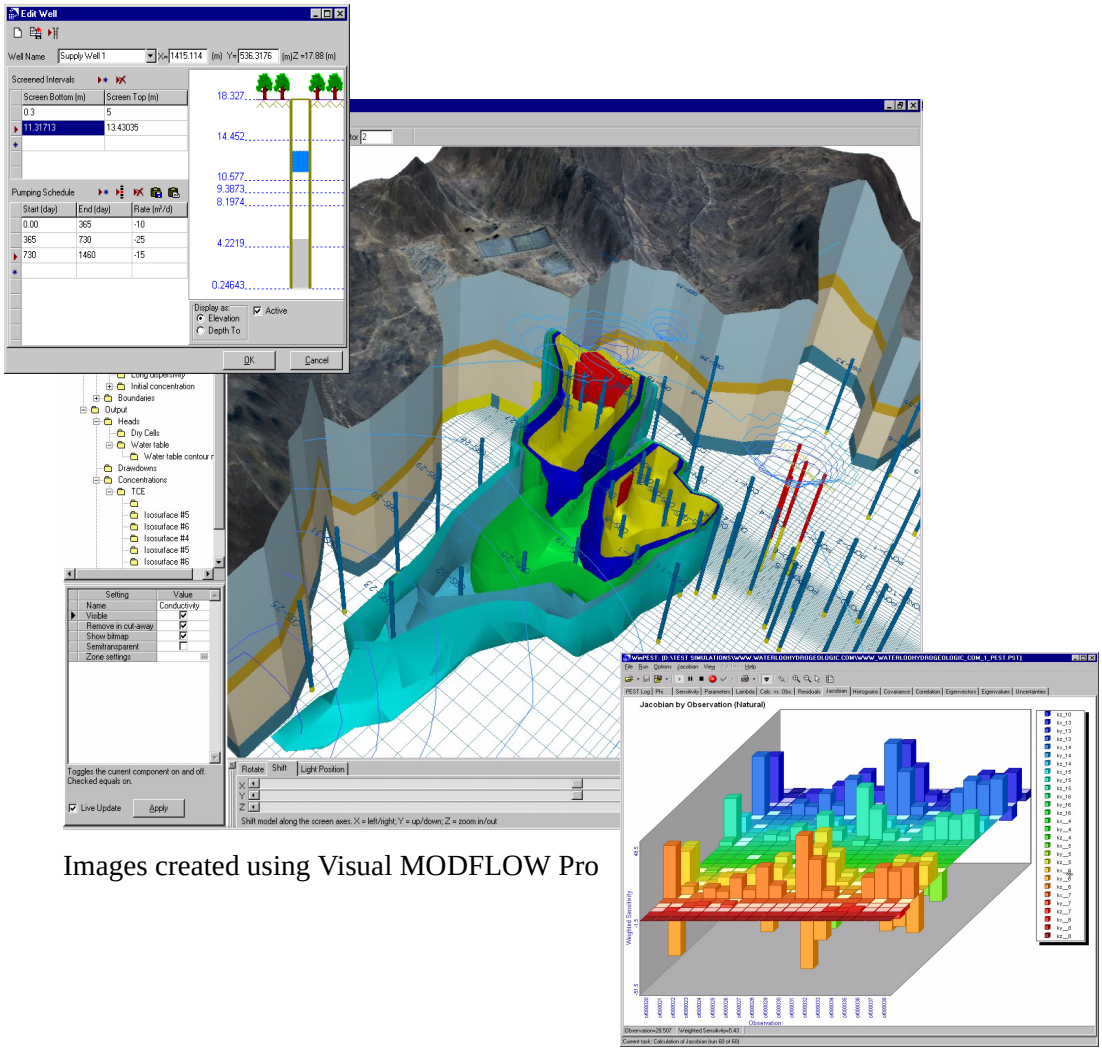
Visual MODFLOW v.3.0
User's Manual

For Professional Applications in Three-Dimensional Groundwater Flow and Contaminant Transport Modeling



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Visual MODFLOW User's Manual

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Visual MODFLOW

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Waterloo Hydrogeologic Inc.

Waterloo Hydrogeologic, Inc. is a recognized leader in the development and application of software for interpreting, analyzing, managing and protecting groundwater resources. Since 1989, Waterloo Hydrogeologic has been developing powerful, yet easy-to-use, software to meet the advanced technology requirements of groundwater and environmental professionals. Today, with over 10,000 registered installations in 90 different countries, Waterloo Hydrogeologic software products are used and approved by consultants, regulators and educators worldwide.

How to Contact WHI

If, after reading this manual and using Visual MODFLOW, you would like to contact Waterloo Hydrogeologic Inc. with comments, suggestions, or if you need technical assistance on how Visual MODFLOW works, you can reach us at:

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Our technical support hours are 9:00 p.m. to 5:00 p.m. EST. Monday to Friday. To help us handle your problem as quickly as possible, please carefully read the following section.

Obtaining Technical Support

Waterloo Hydrogeologic, Inc. provides technical support to registered users of Visual MODFLOW to assist you in dealing with technical problems or difficulties you encounter while using the software. While we try to make the software as easy-to-use as possible, and we take great care in designing the documentation to be comprehensive and easy-to-read, we also recognize that this software is highly specialized and technically complex by it's very nature. As a result, **there may be situations you encounter where the software does not behave as you would expect and you cannot find an appropriate explanation in the documentation**. This type of situation may require you to seek assistance from a technical support specialist.

Technical support is intended as a support service for helping our clients effectively use the software and successfully complete their projects. A valid technical support issue deals with problems you are encountering with the functionality of the software. For advice on numerical modeling (e.g. how to select the model domain, how to design the model grid, which boundary conditions are most appropriate, model solution convergence problems, etc.) please inquire about **Extended Modeling Support Service**.

Waterloo Hydrogeologic also offers numerous open-enrolment groundwater modeling training courses and specialized in-house training seminars. Please visit the Waterloo Hydrogeologic web site for more information.

Generally, we reply to all valid technical support questions within one business day, however please allow up to two business days for a response if a review of your model data is required.

When requesting technical support assistance please be prepared to provide the following information:

- Name of registered user
- Company and office location
- Telephone and fax numbers
- E-mail address
- Product serial number
- Product version number
- Detailed description of the problem you are encountering

The version number can be found using the **Help/About Visual MODFLOW** on the top menu bar.

If your question is of a "How do I...?" type, the above information is generally sufficient. However, if you are reporting a bug (especially one that causes a system crash) or are having technical problems with the program please provide the following additional information:

- Current hardware setup
- Operating system you are using (Win95/Win98/WinNT)
- Amount of RAM that you have on your system
- Amount of free hard disk space remaining on your machine
- Detailed description of when and how the problem occurs

If we are unable to reproduce your problem, or are otherwise unable to solve it, we may ask you to send us a copy of your project files.

Suggested Reference Books

A list of books that may useful for hydrogeology theory and applications are listed below. The full bibliographic references are included in the **Bibliography** section.

- Applied Ground Water Modeling: Simulation of Flow and Advective Transport, Anderson, M.D. and W.W. Woessner, 1992.
- Physical and Chemical Hydrogeology, Domenico, P.A. and F.W Schwartz, 1990.
- Applied Hydrogeology; 3rd edition, Fetter, C.W. Jr., 1994.
- Practical Applications of Groundwater Models, National Ground Water Association, published Biannually.
- ASTM Standard on Analysis of Hydrologic Parameters and Ground Water Modeling, ASTM, 1996.

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WHI Training and Consulting

Waterloo Hydrogeologic Inc. offers both individually tailored and open-enrollment training courses in groundwater flow and contaminant transport modeling.

Waterloo Hydrogeologic also has a professional consulting division specializing in groundwater flow and contaminant transport modeling and geo-environmental database management and analysis.

Other Products by WHI

At WHI we are continually improving our existing products and developing new and innovative software products to meet the advancing technology requirements of groundwater and environmental professionals around the world. The following is a brief description of some other software products developed and distributed by Waterloo Hydrogeologic, Inc.

AquaChem

AquaChem is a fully-integrated software package developed specifically for graphical and numerical analysis of geochemical data sets. It features a powerful database of common geochemical parameters and automated calculations, a comprehensive selection of 13 different geochemical data plotting techniques, and a built-in interface to PHREEQC geochemical modeling.

AquiferTest

The most complete and easy-to-use software package for graphical analysis and reporting of pumping test and slug test analysis data. It comes with a comprehensive selection of built-in solution methods for estimating transmissivity, hydraulic conductivity and storage properties for confined, unconfined, leaky and fractured rock aquifers.

FLOWPATH II

The next generation of powerful, yet easy-to-use software for simulating steady-state groundwater flow with pathlines and contaminant transport. It computes hydraulic heads, pathlines, travel times, velocities and water balances (verified against the USGS MODFLOW, approved by the US EPA, and recommended by the IGWMC).

Visual Groundwater

Visual Groundwater is the one 3-D visualization software package that any groundwater and environmental professional can use to deliver high-quality, three-dimensional presentations of subsurface characterization data and groundwater modeling results.

Visual HELP

Visual HELP is the most advanced hydrological modeling environment available for designing landfills, predicting leachate mounding and evaluating potential leachate seepage to the groundwater table. Visual HELP combines the latest version of the HELP model (Hydrologic Evaluation of Landfill Performance model v.3.07) with an easy-to use interface and powerful graphical features for designing the model and evaluating the modeling results.

WHI Unsat Suite Plus

The WHI UnSat Suite is a fully-integrated software package that combines the most popular and widely-used models for simulating one-dimensional groundwater flow and contaminant transport in the unsaturated zone (includes SESOIL, VS2DT, VLEACH, PESTAN and the HELP model). These models have all been compiled and optimized to run as native Windows applications and are seamlessly integrated within the WHI UnSat Suite graphical modeling environment.

We want your feedback…

At Waterloo Hydrogeologic Inc., we are dedicated to providing a product that is tailored to our customers' needs. Therefore, we are very interested in your thoughts on Visual MODFLOW and welcome your suggestions and comments. We cannot promise to include all your suggestions in the next release, but you have our assurance that all suggestions will be carefully considered. Please indicate a priority or an importance ranking for each of your suggestions.

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1

Introduction to Visual MODFLOW

Visual MODFLOW is the most complete and easy-to-use modeling environment for practical applications in three-dimensional groundwater flow and contaminant transport simulations. This fully-integrated package combines MODFLOW, MODPATH, ZoneBudget, MT3Dxx/RT3D, and WinPEST with the most intuitive and powerful graphical interface available. The logical menu structure and easy-to-use graphical tools allow you to:

- easily dimension the model domain and select units,
- conveniently assign model properties and boundary conditions,
- run the model simulations (MODFLOW, MODPATH, ZoneBudget, MT3D/RT3D, and WinPEST are seamless integrated),
- calibrate the model using manual or automated techniques, and
- visualize the results using 2D or 3D graphics

The model input parameters and results can be visualized in 2D (cross-section and plan view) or 3D at any time during the development of the model or the displaying of the results. For complete three-dimensional groundwater flow and contaminant transport modeling, Visual MODFLOW is the only software package you will need.

When you purchase Visual MODFLOW, or any Waterloo Hydrogeologic software product, you not only get the best software in the industry, you also gain the reputation of the company behind the product, and professional technical support for the software from our team of qualified groundwater modeling professionals. Waterloo Hydrogeologic has been developing groundwater software since 1989 and our software is recognized, accepted and used by more than 10,000 groundwater professionals in over 90 different countries around the world. This type of recognition is invaluable in establishing the credibility of your modeling software to clients and regulatory agencies.

New Features In Visual MODFLOW 3.0

The main interface for Visual MODFLOW 3.0 has the much of the same user-friendly look and feel as the previous versions of Visual MODFLOW, but what's "under the hood" has been dramatically improved to give you more powerful tools for entering, modifying, analyzing and presenting your groundwater modeling data. Some of the more significant upgrade features are described below.

Support for MODFLOW-2000

Visual MODFLOW 3.0 supports the MODFLOW-2000 Groundwater Flow Process for running the flow simulations, but it does not yet support all of the new features and analysis capabilities of MODFLOW-2000 including the Observation Process, the Sensitivity Process and the Parameter Estimation Process. However, Visual MODFLOW does support WinPEST, a more powerful and more robust parameter estimation program.

Support for RT3D Version 2.5

Visual MODFLOW supports and includes Battelle's RT3D Version 2.5 (released in January 2002) for state-of-the-art reactive transport modeling. This latest version of RT3D contains significant improvements to the performance and analysis capabilities including a third-order total-variation diminishing advection solver, an iterative generalized conjugate gradient solver, and cell-by-cell sorption terms. These new solvers can decrease the often excessive run-times by a factor of 10 or more.

Support for the Stream Routing Package

Visual MODFLOW 3.0 support the Stream Routing Package using a Grid-Independent Boundary Object approach. This approach allows Stream Segments to be delineated throughout the model domain using grid-independent line objects. These Stream Segments can be linked together at nodes to create a network of inter-connected Stream Segments. Visual MODFLOW automatically numbers the Segments in downstream order and prompts for the Stream attributes for each segment. The grid cells corresponding to the location of the Stream Segments will be assigned these Stream attributes. If changes are made to the model grid, the grid cells corresponding to the location of the Stream Segments will be re-calculated.

Support for Algebraic Multigrid Solver

Visual MODFLOW supports the Link-Algebraic Multigrid (LMG) Package provided with MODFLOW-2000 and documented in the U.S. Geological Survey Open-File Report 01-177 (Mehl and Hill, 2001). The LMG Package links MODFLOW-2000 with an advanced technique for solving matrix equations, the freeware algebraic multigrid (AMG) solver produced by the GMD - German National Research Center for Information Technology. The LMG Package has some distinct advantages over other

solvers available with MODFLOW-2000 for problems with large grids (more than about 40,000 cells) and (or) a highly variable hydraulic-conductivity field. Testing conducted by the U.S. Geological Survey indicate that execution times using the AMG solver may be 2 to 25 times faster than execution times using MODFLOW's PCG2 Package with the modified incomplete Cholesky pre conditioner. The drawback to the AMG method used in the LMG Package is that is may require 3 to 8 times more memory than PCG2.

Importing and Interpolating Model Property Values

Visual MODFLOW 3.0 imports model property values from discrete data points and interpolates these values to the model grid such that each grid cell has a unique property value. Model property data can be imported from ASCII text files, spreadsheets, or GIS shape files (point or line formats). The 2D interpolation methods currently available include Inverse Distance, Kriging, and Natural Neighbor. For visualization purposes, grid cells may be grouped together in zones representing a user-defined range of property values. The property distribution can be imported to an entire layer, a range of layers, or into a set of existing property zones.

Object-Oriented Boundary Conditions

Visual MODFLOW 3.0 treats the group of cells containing related boundary condition data as a "boundary condition object", such that all of the attributes for a selected group of cells can be modified together. A boundary condition object is created each time a boundary condition is assigned to a group of cells, and each object can be given an alpha-numeric description for easy identification.

Mathematical Operations using Array Variables

A built-in mathematical formula interpreter allows selected model variables to be defined using mathematical formulas containing array variables from other model parameters. For example, if a River boundary condition is assigned using a line object, the Riverbed Conductance can be calculated using the formula:

$COND = $RCHLEN*$RBWIDTH*$K/$RBTHICK

Where:

$COND	= Riverbed Conductance in each cell along the line
$RCHLEN	= Reach Length of the river in each cell along the line
$K	= Vertical Hydraulic Conductivity of the riverbed
$RBTHICK	= Riverbed Thickness in each cell along the line

Another example of the usefulness of this feature is for using the Drain boundary as a seepage face. If the ground surface is not flat (is it ever?) then it is quite tedious to assign the drain elevations for each cell equal to the top of the grid cell elevation.

However, with Visual MODFLOW 3.0 the drain elevation can be defined for all cells in a polygon using the formula:

$DRAIN = $BOT+$DZ

Where:

$DRAIN = Drain Elevation for each cell in the polygon

$BOT = Bottom of cell elevation for each cell in the polygon

$DZ = Thickness of each cell in the polygon

New Overlay Control

The Overlay Control feature has been completely re-designed to make it easier to modify the display settings and viewing priority of the overlays. The Overlay Control also now remembers the most recent Output display settings each time the simulation results are viewed. This avoids the time-consuming and tedious task of re-creating the overlay settings each time the Output data is viewed.

Grid Refinement Error Trapping

Grid refinement is often necessary after the model has been created and run several times. However, the process of adding and moving layer elevations may create invalid boundary condition data where grid cells contain head value less than the bottom elevation of the grid cell. Visual MODFLOW now issues a warning message if the attempted grid modifications will create invalid boundary condition data, and the warning message will provide an option to fix the offending grid cells.

New Features in Visual MODFLOW 3D-Explorer

The Visual MODFLOW 3D-Explorer has also been improved with the addition of several new features and enhancements including:

- Animation sequence pausing, looping and recording to an AVI file
- Light source position control
- Enhanced contour label positioning and controls.
- Concentration plumes are automatically clipped above the water table surface
- Revised project data structure to more closely resemble Visual MODFLOW

1.1 Visual MODFLOW Installation

Hardware Requirements

To run Visual MODFLOW you will need the following minimum system configuration:

- Pentium II, 300 MHz (or equivalent)
- 64 MB of RAM (128 Mb recommended)
- CD ROM drive
- 100 MBytes free disk space;
- Windows 95/98/2000/NT 4.0 (Service Pack 3).

If you have any problems with your particular system configuration, please make sure that you followed the installation instructions precisely (see below in **Installing Visual MODFLOW**). If the problem is still unresolved, contact your hardware experts. Finally, if you are still having trouble, see the section in the Preface on **How to Contact WHI**.

Windows 95/NT Swap File

Windows 95/NT manages the systems virtual memory. To change these settings please see your system administrator.

Installing Visual MODFLOW

Visual MODFLOW must be installed on your hard disk or network disk to run. Please read the section on hardware requirements at the beginning of this chapter to ensure that your system meets the requirements before performing the installation. The **SETUP32.EXE** executable file is used to install Visual MODFLOW on computers using Windows 95/98/2000/NT 4.0 operating systems.

The installation procedure is outlined in the Visual MODFLOW Installation Guide and on the Visual MODFLOW Installation CD-ROM in the directory **Network Instructions / Network Installations**. Please refer to one of these documents before proceeding with the installation.

Starting Visual MODFLOW

Once Visual MODFLOW has been installed on your computer, simply double-click on the Visual MODFLOW 3.0 shortcut icon or click on **Start/Programs/WHI Software/ Visual MODFLOW 3.0/Visual MODFLOW 3.0**.

1.2 About the Interface

The Visual MODFLOW interface has been specifically designed to increase modeling productivity and decrease the complexities typically associated with building three-dimensional groundwater flow and contaminant transport models. In order to simplify the graphical interface, Visual MODFLOW is divided into three separate modules:

- The **Input** section
- The **Run** section
- The **Output** section.

Each of these modules is accessed from the **Main Menu** when a Visual MODFLOW project is started or an existing project is opened. The **Main Menu** serves as a link to seamlessly switch between each of these modules to define or modify the model input parameters, run the simulations, calibrate the model, and display results.

The **Input** section allows the user to graphically assign all of the necessary input parameters for building a three-dimensional groundwater flow and contaminant transport model. The input menus represent the basic "model building blocks" for assembling a data set for MODFLOW, MODPATH, ZoneBudget, and MT3D/RT3D. These menus are displayed in the logical order to guide the modeler through the steps necessary to design a groundwater flow and contaminant transport model.

The **Run** section allows the user to modify the various MODFLOW, MODPATH, MT3D/RT3D, and WinPEST parameters and options which are run-specific. These include selecting initial head estimates, setting solver parameters, activating the re-wetting package, specifying the output controls, etc. Each of these menu selections has default settings, which are capable of running most simulations.

The **Output** section allows the user to display all of the modeling and calibration results for MODFLOW, MODPATH, ZoneBudget, and MT3D/RT3D. The output menus allow you to select, customize, and overlay the various display options for presenting the modeling results.

Getting Around In Visual MODFLOW

The **Main Menu** screen contains the following options:

File	Select a file utility or exit Visual MODFLOW.
Input	Design, modify and visualize the model grid and input parameters.
Run	Enter or modify the model run settings and run the numerical simulations in either project mode or batch mode.

Output Visualize the model output (simulation results) using contour maps, color maps, velocity vectors, pathlines, time-series graphs, scatter plots, etc.

Setup Select the “numeric engine” for both the flow and transport simulation(s).

Help Get general information on how to use Visual MODFLOW.

A Microsoft compatible mouse perform as follows:

Left button: This is the regular ‘click’ button. By holding it down on top of an input box and dragging the mouse, it will also highlight the characters that will be overwritten by the next typed character.

Right button: This button has different functions depending on the context. For example, it closes polygons or ends a line during the assignment of properties, boundaries, etc. During grid design, it also locates grid rows or columns on precise co-ordinates. Using the right button brings up a sub-menu to copy, paste, delete etc.

The **<Alt>** shortcut keys can be used to access toolbar items and to select many buttons and can be used anytime an item or button text has an underlined letter. Simply press the **<Alt>** key and the letter key at the same time to access the item or select the button. The number and letter keys are active only when numerical or text input is required; all other keys are ignored by Visual MODFLOW.

The **File** menu options are described below.

Open... Opens an existing Visual MODFLOW data set.

New Creates a new Visual MODFLOW data set.

Save As Saves the current model to a different filename.

Close Closes the current model.

Import MODFLOW Imports an existing set of MODFLOW data files (*.BAS);

Export... Exports the model image to a graphics file (AutoCAD .DXF or (*.DXF) or an Enhanced Windows Metafile (*.EMF).

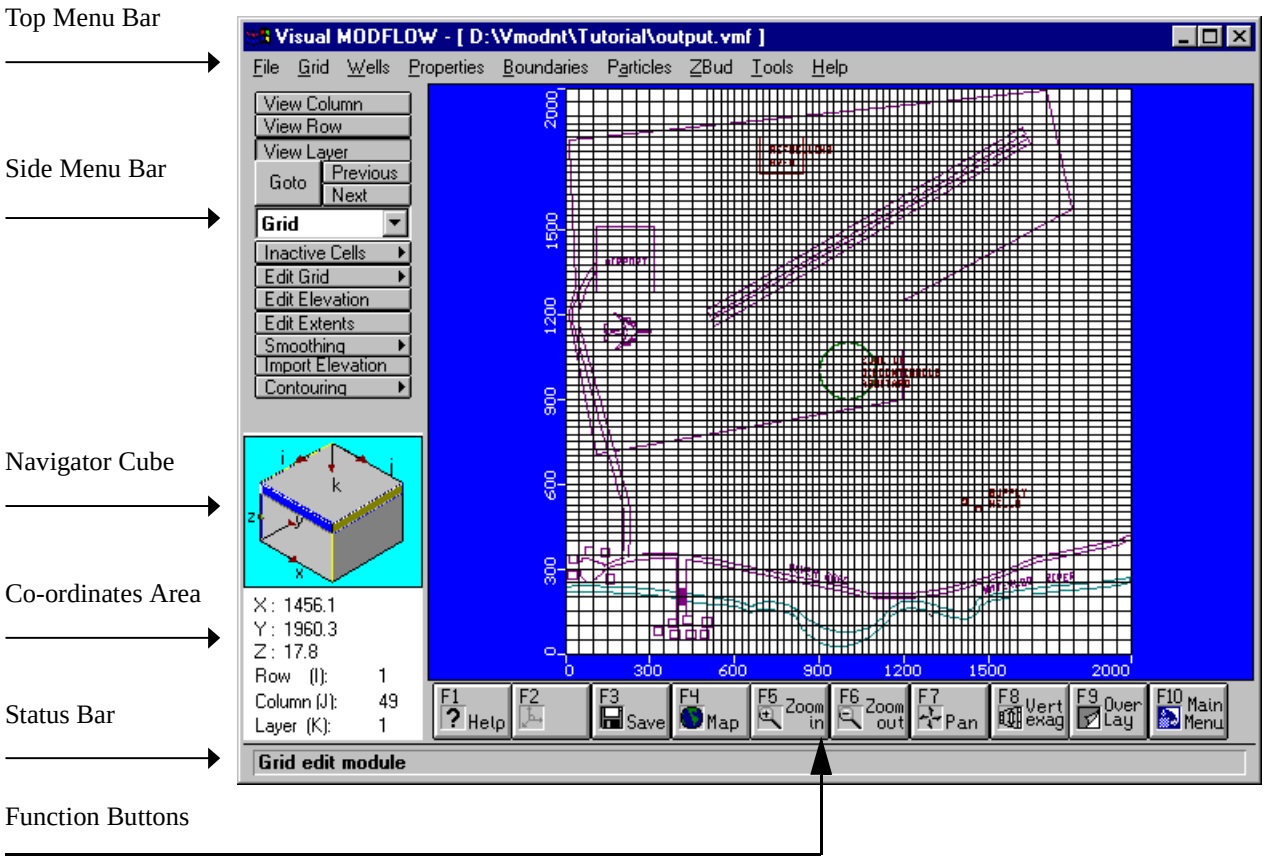
Change Units... Changes units in the current model (but does NOT convert the existing data values).

Print Prints the model display area to the selected printer (with or without a description of the image).

eXit Closes the project and shut-down Visual MODFLOW.

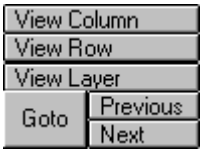
Screen Layout

After opening a Visual MODFLOW project and selecting the Input module, a screen layout similar to the figure below will appear.



Top Menu Bar: Contains specific data category menus for each section of the interface (**Input**, **Run** and **Output**).

Side Menu Bar: Contains the **View** Control buttons plus tool buttons specific for each data category. The view options are as follows:



[View Column] View a cross-section along a column.

[View Row] View a cross-section along a row.

[View Layer] Switch from cross-section to plan view.

[Goto] View a specified column, row or layer.

[Previous] View previous column, row, or layer.

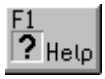
[Next] View next column, row, or layer.

Navigator Cube: Provides a simplified 3D representation of the model domain highlighting the current layer, column and row being viewed.

Co-ordinates Area: Shows the current location of the cursor in model co-ordinates, and shows the current cell indices on which the cursor is located.

Status Line: Describes the functionality and use of the feature currently highlighted by the cursor.

Function Buttons: Common functions to the **Input**, **Run**, and **Output** screens can be selected by clicking on the button or by pressing the function key on your keyboard. The function buttons are:



[F1-Help] Opens the general help window.

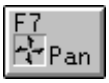
[F2-3D] Opens the Visual MODFLOW 3D-Explorer.

[F3-Save] Saves the current data for the model.

[F4-Map] Import and display .DXF site map files.

[F5–Zoom In] Enlarge the display of a selected rectangular area.

[F6–Zoom Out] Resets the display area to show the entire model domain.



[F7-Pan] Drag the current view of the model in any direction to display a different model region.

[F8–Vert Exag] Set the vertical exaggeration value for viewing cross-sections along a row or column.

[F9-Overlay] Opens the **Overlay Control** window to make selected overlays visible and to customize the priority (order) in which they appear.

[F10–Main Menu] Returns to the **Main Menu** screen.

The interface features described above are consistent throughout the entire Visual MODFLOW interface. The tool buttons and options available on the Side Menu Bar (see above figure) will change depending on the active data category in the **Input** and **Output** screen. For example, the tool buttons shown on the Side Menu bar in the above figure pertain to the **Grid** module, for designing and modifying the finite difference model grid. The tool buttons available for the **Properties** module are completely different. The options available for each **Input** and **Output** data category are described in the appropriate sections of this document, and instructions for using some of these options is described in the tutorial exercise document (**Tutorial.pdf**) provided on installation CD-ROM.

1.3 Visual MODFLOW Project Files

Each Visual MODFLOW project consists of many different data files, each pertaining to a specific component of the model (e.g. model setup, grid data, flow boundary conditions, flow properties, particle locations, etc.), whereby each data file is distinguished by the file extension. For example:

- *projectname.VMF* - general model information
- *projectname.VMG* - model grid information
- *projectname.VMP* - flow model properties information
- *projectname.VMB* - flow model boundary condition information
- *projectname.VMW* - flow model pumping/injection well information
- *projectname.VMO* - flow model observation well information
- projectname.*VMA* - flow model particle locations (for MODPATH)

A detailed listing of each Visual MODFLOW project file is provided in Appendix A along with a description of the data structure for each file.

Although the data files associated with each Visual MODFLOW project are easily distinguished by the project name prefix, it is strongly recommended to create a separate folder for each modeling project to make it more practical to manage any map files or external data files associated with the project.

Although most of the data files associated with a Visual MODFLOW project are stored in ASCII format, it is not recommended to manually modify or manipulate the data in these files. Visual MODFLOW will not be able to successfully open a project if it encounters any unexpected or incorrect file formats in any of the data files related to the project.

That being said, the reason these files are stored in ASCII format, and the reason the data structures are explained in Appendix A is so advanced users would be able to generate their own Visual MODFLOW data sets using their own specialized programs and utilities. If this is attempted, it is strongly recommended to backup the original data files generated by Visual MODFLOW before replacing or manually modifying them.

2

Getting Started

This chapter presents information on:

- Importing MODFLOW Data Sets
- Creating a New Model
- Selecting Numeric Engines
- Changing Units in an Existing Model
- Using the Overlay Control

2.1 Importing MODFLOW Data Sets

In some situations it may be necessary to import an existing MODFLOW data set into Visual MODFLOW in order to review the model or evaluate different scenarios. Visual MODFLOW can import existing MODFLOW data sets provided they are in MODFLOW-88 format.

When importing MODFLOW data sets, Visual MODFLOW will make the best attempt to re-create the original model from the data present in the MODFLOW files. However, depending on the layer type settings (LAYCON) in the data, the sequence outlined below may vary. **You must check the data set to ensure that all information has been imported correctly**.

To import an existing MODFLOW data set selecting **File/Import MODFLOW** from the **Main Menu** of Visual MODFLOW. A file selection dialog will appear asking for the name of the **.BAS** file from the MODFLOW model. The packages being used for that particular simulation are automatically recognized from the **.BAS** file and the following standard MODFLOW files will be read and the data imported:

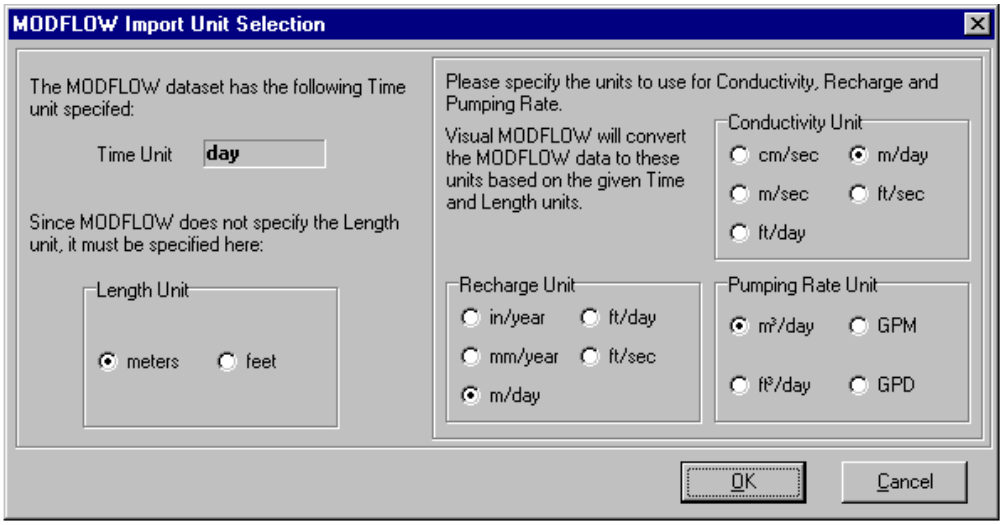
modelname.BAS	*modelname*.BCF	*modelname*.WEL
modelname.DRN	*modelname*.SIP	*modelname*.EVT or .EVP
modelname.GHB	*modelname*.HFB	*modelname*.STR
modelname.RCH	*modelname*.RIV	

where *modelname* must be the same for all files.

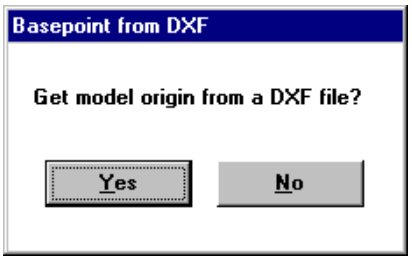
After selecting a *modelname*.BAS file for the MODFLOW model, you will be asked to select a name for the new Visual MODFLOW model, *filename*.VMF. If you chose the same name as the MODFLOW model, all of the original MODFLOW files will be overwritten at translation time.

If any files are missing from your data set, you will be notified and the import procedure will be aborted. Before attempting to import the same data set, please locate or create the necessary files and place them in the same directory as the **.BAS** file. If you do not want to create the files or include them in the import, modify the **.BAS** file and remove the unit numbers for those files.

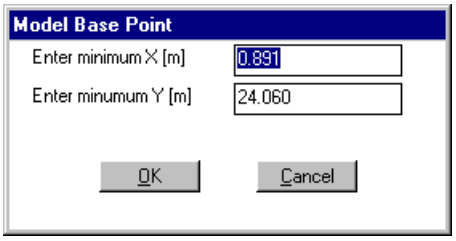
Next, you will be asked to select the model units as shown in the following figure. This is analogous to the unit selection during the creation of a new model. The default time unit is read directly from the original **.BAS** file and all data are read in and stored accordingly. However, the user may modify the units displayed by Visual MODFLOW for the length, conductivity and recharge using the window shown in the following figure.



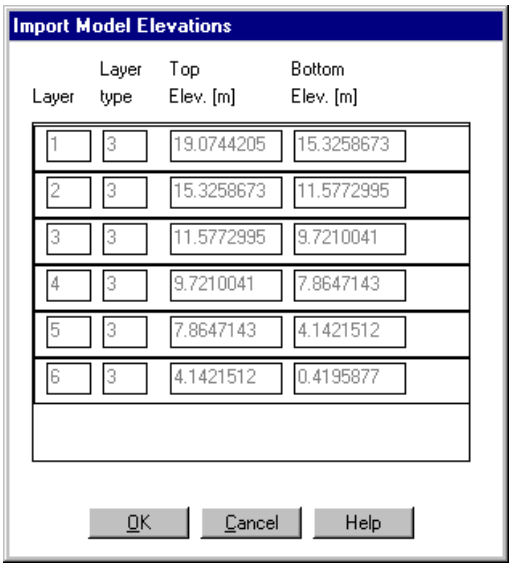
After choosing the model units, you will be prompted with the following window, asking you whether the model base point should be taken from a .DXF file.



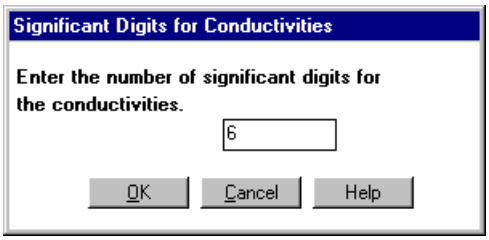
If you answer yes, you will be prompted to select the .DXF file. After selecting a .DXF file, or if you answered **[No]** to the above questions, the following window will appear, asking you to either confirm or input the model base point. The default coordinate values will be either the origin of the **.DXF** file or (0, 0).



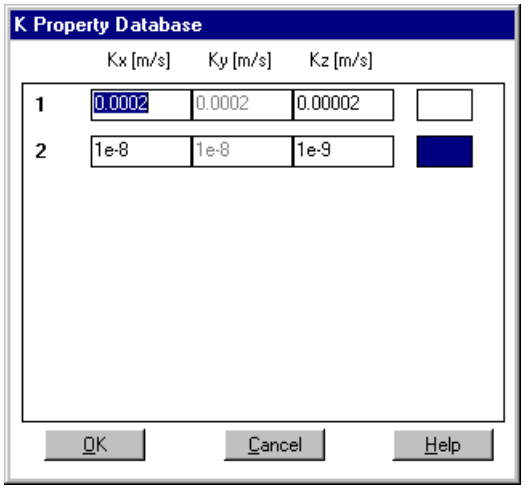
At this point, the Import Utility will ask for the top and bottom elevations of each of the layers. The elevation for layers classified as unconfined (LAYCON = 3) or confined/ unconfined with variable transmissivity (LAYCON = 1) may not be edited here.



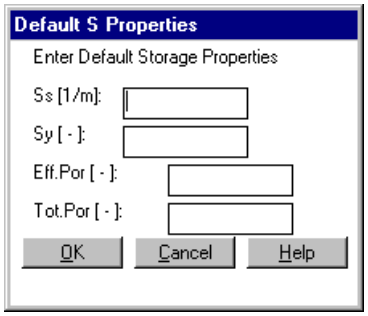
After editing the layer elevations, you will be prompted for the number of significant digits to use for defining the hydraulic conductivity value for each Visual MODFLOW property zone. A low number will import the data faster but will likely create fewer zones with more rounding errors, while a high number may take a while to import the data and will potentially create many zones with smaller rounding errors.



Next you will be asked if you would like to edit or view the conductivity database. If you select **[Yes]**, the **K Property Database** window will appear as shown in the following figure. The conductivities generated are unique values and Visual MODFLOW lists these values with no repetition. The conductivity values should be checked and modified if necessary:



The final step asks for the default values for Specific Storage, Specific Yield, and Porosity. The values for these variables are not imported from the MODFLOW data set and will initially be assigned constant for all layers.



Once the importing procedure is completed, the program will proceed to the **Main Menu**.

Importing Same Cell Boundary Conditions

For certain boundary conditions, MODFLOW accepts multiple cell entries for the same boundary condition, in the same stress period (e.g. general head, rivers, and drains). For the General Head boundary condition, MODFLOW calculates the flux in the cell using the equation:

$$Q = \Sigma Ci(h - hi)$$

where Q = flux in the grid cell

Ci = ith conductance term in the grid cell

h = calculated head in the grid cell

hi = ith reference head in the grid cell

Although Visual MODFLOW does not allow you to assign separate boundary condition values for the same boundary condition in the same cell, it does allow you to import this information from a MODFLOW data set. For example, with the General Head boundary condition Visual MODFLOW will calculate the representative conductance and reference head values using the following formulas:

$$\tilde{C} = \Sigma Ci$$

$$\tilde{h} = \left(\frac{\Sigma CiHi}{\Sigma Ci}\right)$$

Limitations of Importing MODFLOW Data Sets

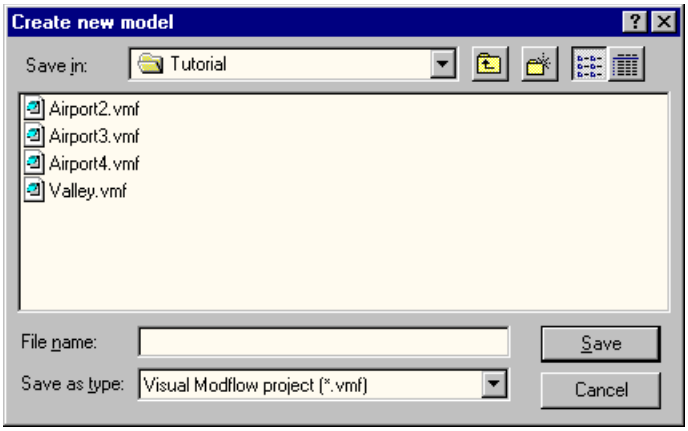
The following list outlines some of the known limitations that exist for importing MODFLOW data sets.

- **Interlayer Leakage** (VCONT) - Visual MODFLOW requires the top and bottom elevations for each grid cell in the model, regardless of the layer type, and it requires hydraulic conductivity values (Kx, Ky and Kz) for each grid cell. Visual MODFLOW uses this information to calculate the interlayer leakage (VCONT) values. As a result, Visual MODFLOW does not store the VCONT values and will essentially ignore the VCONT data from existing MODFLOW data sets. This causes serious problems for existing MODFLOW models where an aquitard layer was ignored and a VCONT value was used to simulate the leakance through the aquitard between two aquifer layers.
- **Layer Bottom Elevations** - MODFLOW-88 and MODFLOW-96 models containing confined layers (LAYCON = 0) or confined/unconfined layers with constant transmissivity (LAYCON=2) do not require or store the grid cell elevation data for these layer types because it was not required for the calculations. If Visual MODFLOW encounters a model with these types of layers, it will prompt the user for the bottom elevation of the layer. For the top layer, the user will also be prompted to input the top elevation. This can cause problems if the layers have a variable bottom elevation. You can minimize the loss of data by re-creating the MODFLOW data set with the layers all set to confined/unconfined with variable transmissivity (LAYCON = 3).
- **Specific Storage, Specific Yield and Porosity** - Specific storage, specific yield and porosity are all set to a single value during the import. These can be modified on a cell-by-cell basis afterwards.
- **Stream Routing Package** - Although the Stream Routing Package is supported by Visual MODFLOW, the grid cell data from the existing MODFLOW model will not be visible because Visual MODFLOW stores the Stream Routing data using grid-independent stream objects and not on a cell-by-cell basis. However, if the Stream Routing Package data file is present in the Visual MODFLOW project directory, and it has the same name as the Visual MODFLOW project, then the Stream Routing Package data file will be used during the MODFLOW calculations (see description below).
- **Aquitard Compressibility Package** - The Aquitard Compressibility Package is not supported by Visual MODFLOW and will be ignored if it is present in the MODFLOW data set.

2.2 Creating a New Model

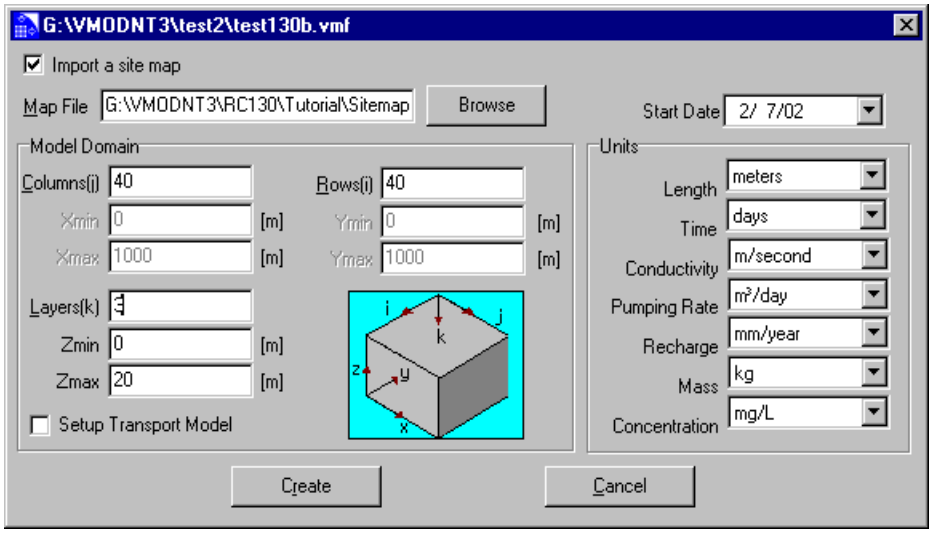
To create a new model, select **File/New** from the **Main Menu** screen of Visual MODFLOW.

A **Create New Model** dialog will appear, as shown below. Select the directory where you want to save the model files and type in the new model name.



Press the **[Save]** button to continue creating the new model. A warning will appear if the operation was unsuccessful (e.g., if the same name already exists).

Next, the Model Setup window will appear as shown below. This window is used to select a **site map**, specify the dimensions of the **Model Domain** and the finite difference grid, and select the **Units** to use for each model data type.



Map File

The **Import a site map** option is used to select a site map to overlay on the model domain. Visual MODFLOW currently supports bitmap files (.BMP) and AutoCAD Drawing eXchange Format (.DXF) files. If this option is selected, use the **[Browse]** button to locate and select the site map to use.

Start Date

The **Start Date** of the model is the date corresponding to the beginning of the simulation time period. Currently, this date is relevant only for transient flow simulations where recorded field data may be imported for defining time schedules for selected boundary conditions (Constant Head, River, General Head and Drain).

Once the model is created, the **Start Date** can be modified by selecting **File/Change Model Units** from the **Main Menu** (see section Changing Model Settings on page 30).

Model Domain

The **Model Domain** section is where the model dimensions and initial grid discretization are defined. The initial grid will have uniform grid cell sizes throughout the entire model, but all grid spacing and elevations are customizable inside of the Visual MODFLOW interface.

- **Columns** is the number of uniformly spaced columns in the model grid.
- **Xmin** is the minimum X coordinate for the model grid
- **Xmax** is the maximum X coordinate for the model grid
- **Rows** is the number of uniformly spaced rows in the model grid
- **Ymin** is the minimum Y coordinate for the model grid
- **Ymax** is the maximum Y coordinate for the model grid
- **Layers** is the number of uniformly spaced layers in the model grid
- **Zmin** is the minimum Z coordinate (elevation) for the model grid
- **Zmax** is the maximum Z coordinate (elevation) for the model grid

If the **Import a site map** option is selected, the **Xmin**, **Xmax**, **Ymin** and **Ymax** fields will be disabled. Otherwise the **Xmin**, **Xmax**, **Ymin** and **Ymax** co-ordinates must be entered. Visual MODFLOW generates a uniform grid based on these dimensions. The uniform grid spacing may be customized in the **Input** section of Visual MODFLOW (see section Gridlines (Rows and Columns) on page 41).

If the **Setup Transport Model** option is selected you will be prompted with the **Setup Transport Numeric Engine** window. For more information on this procedure please refer to the section Mass Transport Numeric Engine on page 25.

Units

One of the major benefits of using Visual MODFLOW is that it is not restricted to consistent units for length and time for all parameters. The **Units** section of this dialog

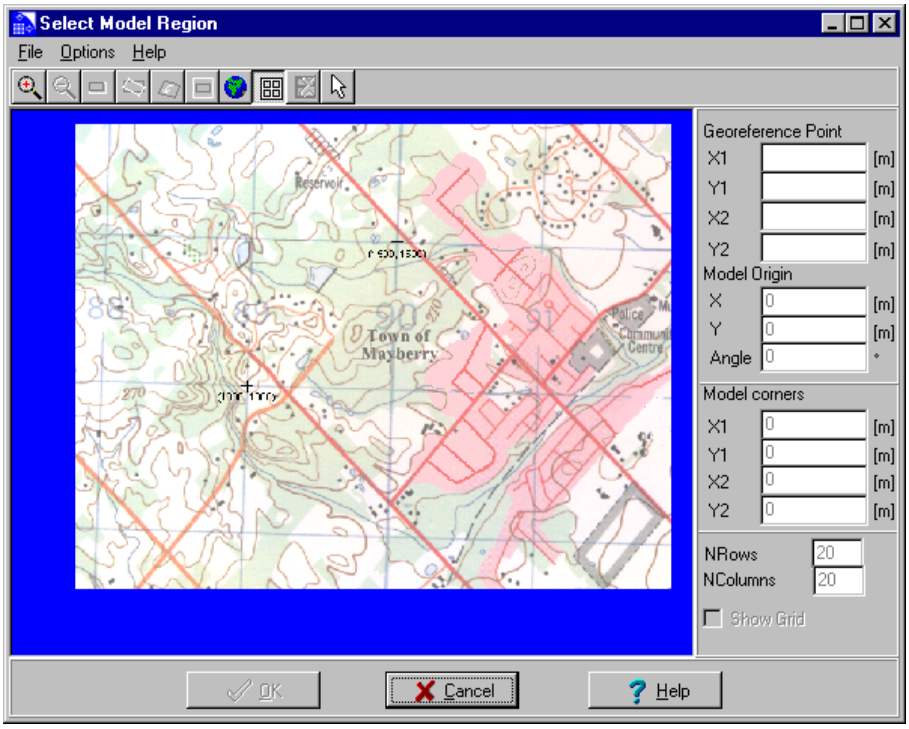
is used to select the desired units for each of the major units categories available in Visual MODFLOW. Each of the unit categories provides a selection of both Imperial units and SI units. With Visual MODFLOW, the units DO NOT need to be consistent between SI and Imperial such that a model may have Hydraulic Conductivity values assigned in units of cm/sec and well pumping rates in US GPM.

Once the model is created, the selected units can be changed by selecting **File/Change Model Units** from the **Main Menu** (see section Changing Model Settings on page 30.

After the desired units have been selected, press the **[Create]** button.

If the **Import a site map** option is NOT selected, the new model data files will be generated and the Visual MODFLOW **Main Menu** will display the model domain. See Chapter 2 for instructions on refining the finite difference grid and assigning the model properties and boundary conditions.

If the **Import a site map** option is selected, a **Select Model Region** window will display the selected base map as shown in the following figure and described in the following sections.



2.2.1 Importing a Site Map

A site map (or base map) of the model region is often useful for gaining a perspective of the dimensions of the model and for locating important characteristics of the model. The base map does not contain and specific data used in the calculations and the presence of a base map does not influence the results of the simulation, but it is helpful for enhancing the visualization of the model. When a model is first created, Visual MODFLOW supports the use of site maps in either AutoCAD .DXF or bitmap .BMP image file formats.

Once the model has been created, a .DXF site map can be added to the model using the **[F4 - Maps]** button in the lower toolbar of the Visual MODFLOW interface.

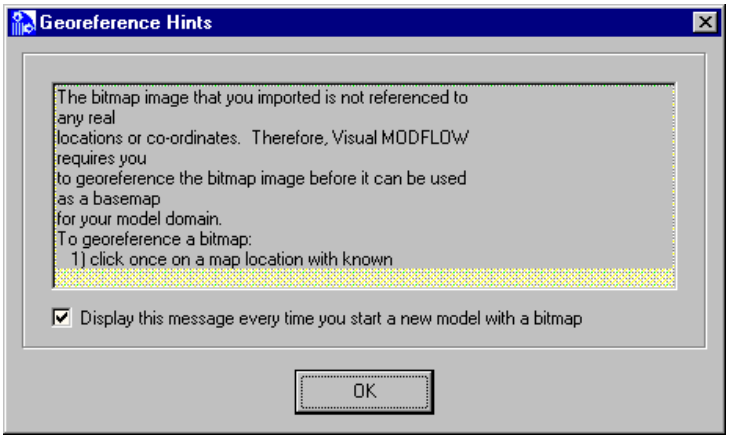
If a bitmap image is being used as the model base map then the bitmap image must first be georeferenced by entering the X-Y world coordinates of two known locations on the image. The georeferencing procedure is described in the following section.

If an AutoCAD file (.DXF) is being used as the model site map, proceed to section Selecting the Model Region on page 21.

Georeferencing a Bitmap

Bitmap image files (.BMP) do not contain any co-ordinate information in their internal file format. Therefore, the .BMP file used as the model site map must be manually georeferenced in order to map a co-ordinate system to the pixels on the image.

The following **Georeference Hints** window will appear with some guidance on how to georeference the bitmap image.


Georeference Hints
The bitmap image that you imported is not referenced to
any real
locations or co-ordinates. Therefore, Visual MODFLOW
requires you
to georeference the bitmap image before it can be used
as a basemap
for your model domain.
To georeference a bitmap:
1) click once on a map location with known
Display this message every time you start a new model with a bitmap
OK

In order to map the pixels of the bitmap image to a world co-ordinate system, the bitmap image must have two georeference points with known world co-ordinates. These georeference points must be defined by the user as described below.

Adding Georeference Points

To set the first georeference point,

- Click the [Set **Georeference Point]** icon in the toolbar

- Click on a map location where the world co-ordinates are known
- A **Georeference point** window will appear prompting for the X and Y world co-ordinates of the selected location
- Enter the X and Y world-coordinates for this point
- Repeat this procedure for the second georeference point

Once the two georeference points have been established, the model domain must be oriented on the model base map as described in the section Selecting the Model Region on page 21.

Deleting Georeference Points

To delete a georeference point,

- Click the **[Delete Georeference Point]** icon in the toolbar

- Click on the georeference point to delete

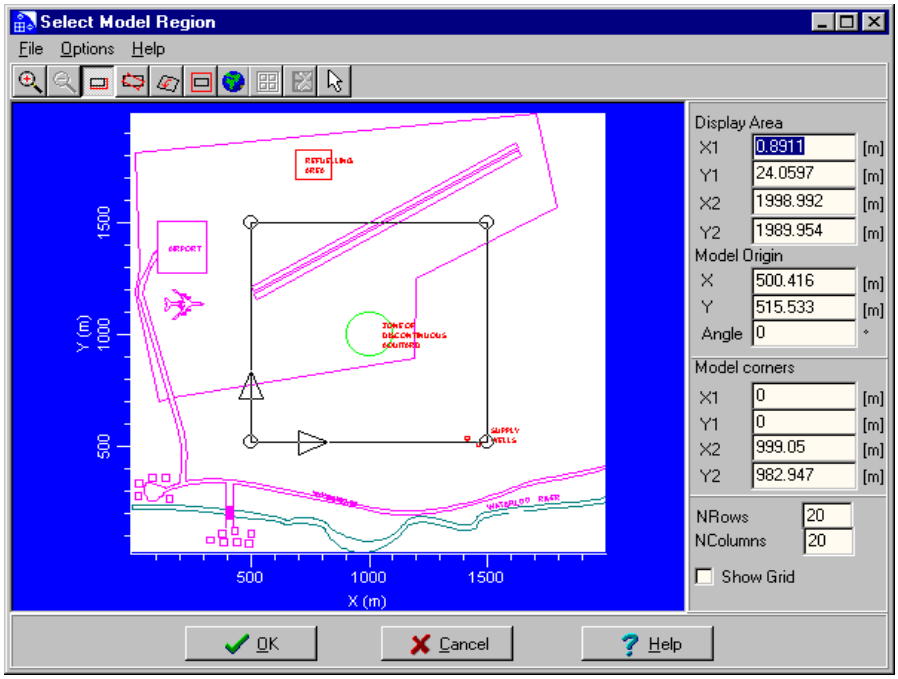
Note: When a georeference point is deleted, a new georeference point must be added.

Loading a New Map File

If the bitmap image is not what was expected, a new bitmap image may be loaded by selecting **File/New Map** from the top menu bar, or by clicking the **[New Map]** icon in the toolbar and selecting the desired bitmap image file.

Selecting the Model Region

The **Select Model Region** window is used to orient the model domain on the base map and specify the region of the base map to use for the model domain. The model domain is represented by an outline of a box with circular nodes at each corner and with arrows pointing along the X and Y axes (see figure below). The model domain box can be shifted, expanded, and rotated to any alignment on the site map using the toolbar options described below.



Zoom In Click-and-drag the mouse to select the zoom area.

Zoom Out View the entire map display area.

Resize Region Click-and-drag a corner of the model domain box to stretch or shrink the size of the model domain. Double clicking on the model region will switch the mode between Resize Region and Rotate Region.

Rotate Region Click-and-drag a corner of the model domain box to rotate and align the model domain. Double clicking on the model region will switch the mode between Rotate Region and Resize Region.

Align Region Align the model domain with the x-axis.

Full Region Enlarge the model domain to the full extents of the base map.

New Map Load a new .DXF or .BMP file for the site map.

If an AutoCAD .DXF file is used for the site map, the top right-hand section will contain the **Display Area** co-ordinates where (**X1**, **Y1**) is the map co-ordinate in the lower left-hand corner and (**X2**, **Y2**) is the map co-ordinate in the top right-hand corner. These values are automatically read from the .DXF file and may be modified to expand or shrink the available 'realestate' for defining the model region.

If a bitmap image .BMP file is used for the site map, the top right-hand section will contain the **Georeference Points** co-ordinates. These values cannot be modified unless one of the georeference points is deleted and a different georeference point is assigned.

The **Angle** is the degree angle of rotation of the model region from the world co-ordinate axes.

The **Model Origin** is the **X** and **Y** world co-ordinate location of the bottom left-hand corner of the model domain.

The **Model corners** are the model co-ordinates of the bottom left-hand corner (**X1**, **Y1**) and the top right-hand corner (**X2**, **Y2**) of the model domain. If the **Angle** is 0.0 and (X1, Y1) is the same as the **Model Origin**, then the model co-ordinate system will coincide with the world co-ordinate system. However, if the model domain is rotated from the world co-ordinate axes, then the model domain will contain dual co-ordinate systems; (1) the world co-ordinate system; and (2) the model co-ordinate system. In this situation it is most practical to set (**X1**, **Y1**) equal to (0, 0), and set (**X2**, **Y2**) equal to the distance in the X and Y directions.

The **NRows** and **NColumns** fields contain the number of finite difference rows and columns, respectively, for the model grid. The **Show grid** switch is used to show/hide the model grid inside the model domain.

Dual Co-ordinate Systems

Visual MODFLOW uses two co-ordinate systems, world co-ordinates and model co-ordinates. This allows the model to be rotated on the site map while maintaining a UTM based co-ordinate system. At any time you are able to view both the world and model co-ordinates of the mouse by opening the cell inspector (please refer to the **Cell Inspector** section, in this Chapter).

Transforming World Co-ordinates to Model Co-ordinates

To transform world co-ordinates to model co-ordinates, use the following formulas. There is no transformation for the Z co-ordinates of the model.

$$X_{model} = (X_{world} - X_{world-origin}) \cdot \cos\theta + (Y_{world} - Y_{world-origin}) \cdot \sin\theta + X_{model-origin}$$

$$Y_{model} = -(X_{world} - X_{world-origin}) \cdot \sin\theta + (Y_{world} - Y_{world-origin}) \cdot \cos\theta + Y_{model-origin}$$

Transforming Model Co-ordinates to World Co-ordinates

$$X_{world} = (X_{model} - X_{model-origin}) \cdot \cos\theta - (Y_{model} - Y_{model-origin}) \cdot \sin\theta + X_{world-origin}$$

$$Y_{world} = (X_{model} - X_{model-origin}) \cdot \sin\theta + (Y_{model} - Y_{model-origin}) \cdot \cos\theta + Y_{world-origin}$$

Where;

X_{model}	= displayed X model co-ordinate
$X_{model-origin}$	= model X start point (bottom left corner)
X_{world}	= displayed X world co-ordinate
$X_{world-origin}$	= world X start point (bottom left corner)
Y_{model}	= displayed Y model co-ordinate
$Y_{model-origin}$	= model Y start point (bottom left corner)
Y_{world}	= displayed Y world co-ordinate
$Y_{world-origin}$	= world Y start point (bottom left corner)
θ	= angle of rotation

2.3 Selecting Numeric Engines

Visual MODFLOW supports all of the most recent public domain and proprietary versions of MODFLOW and MT3D for simulating groundwater flow modeling and mass transport modeling, respectively. In Visual MODFLOW, these programs are referred to as Numeric Engines because they perform the numeric calculations required to solve the finite difference equations of groundwater flow and mass transport.

Although the most recent versions of these programs are going to be used the majority of the time, the reason for continuing to support the legacy codes is to give the user the

opportunity to reproduce simulation results from older model data sets using exactly the same simulation programs.

> **Note:** The MODPATH and Zone Budget versions included in Visual MODFLOW are the latest U.S.Geological Survey versions, compiled and optimized to run as 32 bit native Windows applications.

The numeric engines used for the a model can be selected from the **Main Menu** of Visual MODFLOW by clicking **Setup/Numeric Engines** from the top menu bar and choosing either **Flow** or **Transport** as described in the following sections.

2.3.1 Groundwater Flow Numeric Engine

Visual MODFLOW provides a selection of two numeric engines for simulating groundwater flow:

- MODFLOW-96 (Public Domain, U.S. Geological Survey)
- MODFLOW-2000 (Public Domain, U.S. Geological Survey)

By default, all new models created with Visual MODFLOW will use MODFLOW-2000 as the numeric engine for groundwater flow.

A brief description of the differences between these numeric engines is provided in Appendix C while a more detailed explanation of the differences is provided in the MODFLOW-2000 Reference Manual provided in the Manuals folder on the Visual MODFLOW installation CD-ROM.

In terms of the Visual MODFLOW interface, the differences between these two numeric engines is very subtle, with the exception that MODFLOW-2000 has built-in parameter estimation capabilities (not yet supported by Visual MODFLOW).

2.3.2 Mass Transport Numeric Engine

Visual MODFLOW currently provides a selection of six different numeric engines to use for the mass transport model as listed below:

- MT3Dv1.5 (Public Domain, U.S. Dept. of Defence)
- MT3D96 (Proprietary, S.S. Papadopulos & Associates, Inc.)
- MT3DMS (Public Domain, U.S. Army Corp of Engineers)
- MT3D99 (Proprietary, S.S. Papadopulos & Associates, Inc.)
- RT3Dv1.0 (Public Domain, Battelle Northwest Laboratories)
- RT3Dv2.5 (Public Domain, Battelle Northwest Laboratories)

By default, all new models created with Visual MODFLOW will use MT3DMS as the mass transport numeric engine.

All of the different mass transport programs supported by Visual MODFLOW have evolved from essentially the same version of MT3D (Mass Transport in 3 Dimensions)

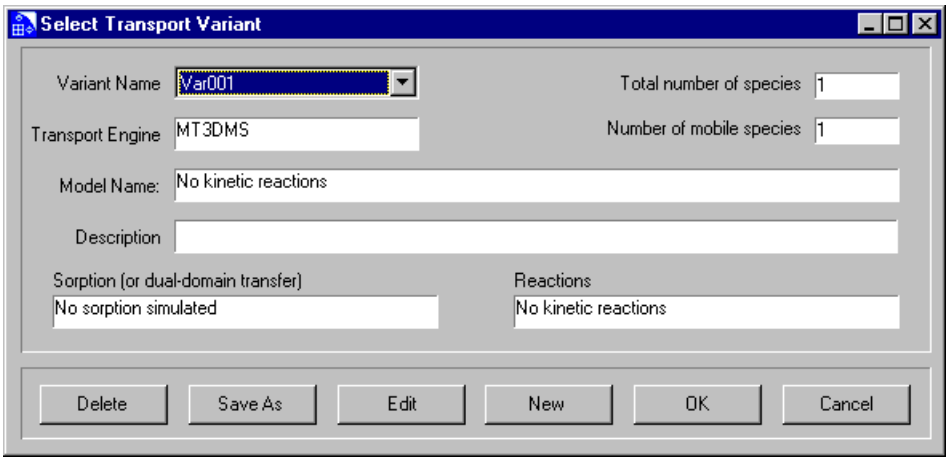
first developed by Chunmiao Zheng in 1990 at S.S. Papadopulos & Associates, Inc. with partial support from the U.S. Environmental Protection Agency (USEPA).

The differences between the various Transport Numeric Engines are primarily rooted in the options for specifying options for sorption, reactions and solvers. A brief description of the different options available from each of the available mass transport numeric engines is provided in Appendix C. A more detailed description of the analysis capabilities for each program can be found in the reference manuals provided in the **Manuals** folder of the Visual MODFLOW installation CD-ROM.

Defining Transport Variants

Due to the number of different Mass Transport numeric engines available and the different simulation capabilities associated with each one, Visual MODFLOW stores all of the transport characteristics for a model (e.g. numeric engine, observations, properties, and boundary conditions) in a compressed file called a Transport Variant. As a result, each Visual MODFLOW model may have several different Transport Variants associated with the same flow model. This allows more efficiency for managing the mass transport calibration and analysis.

To select the desired Numeric Engine for the Mass Transport model, select **Setup/ Numeric Engines/Transport** from the **Main Menu**. The following **Select Transport Variant** window will appear.



This window contains a summary of the basic information for the current Transport Variant. A different Transport Variant may be selected from the **Variant Name** field. The buttons along the bottom of the dialog function as follows:

[Delete] Deletes the selected variant

[Save As] Create a new variant with the current variant settings

[Edit] Modify the selected variant

[New] Creates a new variant with default settings.

[OK] Accepts the selected variant and returns to the **Main Menu**

[Cancel] Returns to the **Main Menu** without changing the variant.

In Visual MODFLOW the Transport Variant information is saved in the *project.vmf* file. For each variant a file called *project.var001* is saved to the working directory where *var00#* is the variant number. When entering species specific information in the **Input** section, the files containing the transport information are created in the working directory. When a new variant is created the current information from the Input Module is compressed and saved to the *project.var00#* file. All species specific information in **Input** will be reset for the new variant to the default values entered in the Transport Engine Options dialog. As you move between your variants, the input and output for the variants is compressed and uncompressed to and from the variant repositories.

The reason for this data structure is to allow multiple scenarios for contaminant transport using the same flow model. This allows different remediation alternatives to be examined given an identical set of flow conditions.

Modifying a Transport Variant

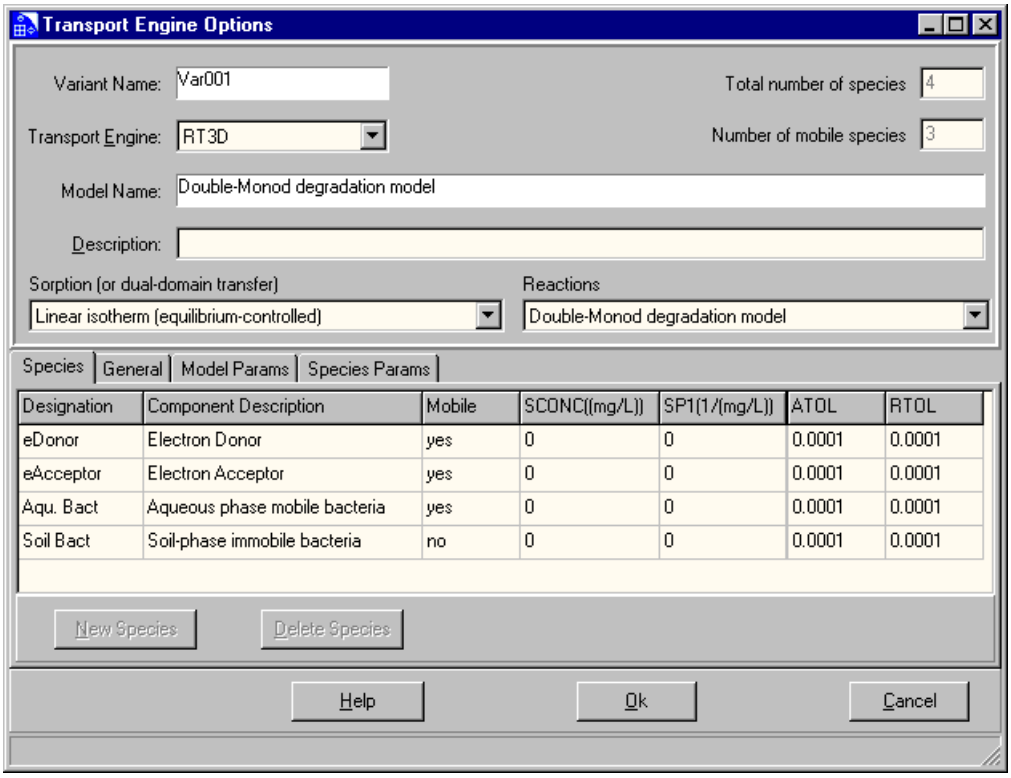
To modify the selected Transport Variant, press the **[Edit]** button and the following **Transport Engine Options** window will appear.

The **Transport Engine Options** window is used to:

- Modify the Transport Engine
- Modify the Sorption method
- Modify the Reaction method

The available **Sorption** and **Reaction** options will vary depending on which Transport Engine is selected. A comparison of the various sorption and reaction options available for each Transport Engine is provided in Appendix C.

Note: The **Transport Engine Options** window is used only to initialize the transport property values. Once the Transport Variant has been selected, the **Transport Engine Options** window can NOT be used to modify the sorption and reaction parameter values (i.e. any changes made will be ignored).

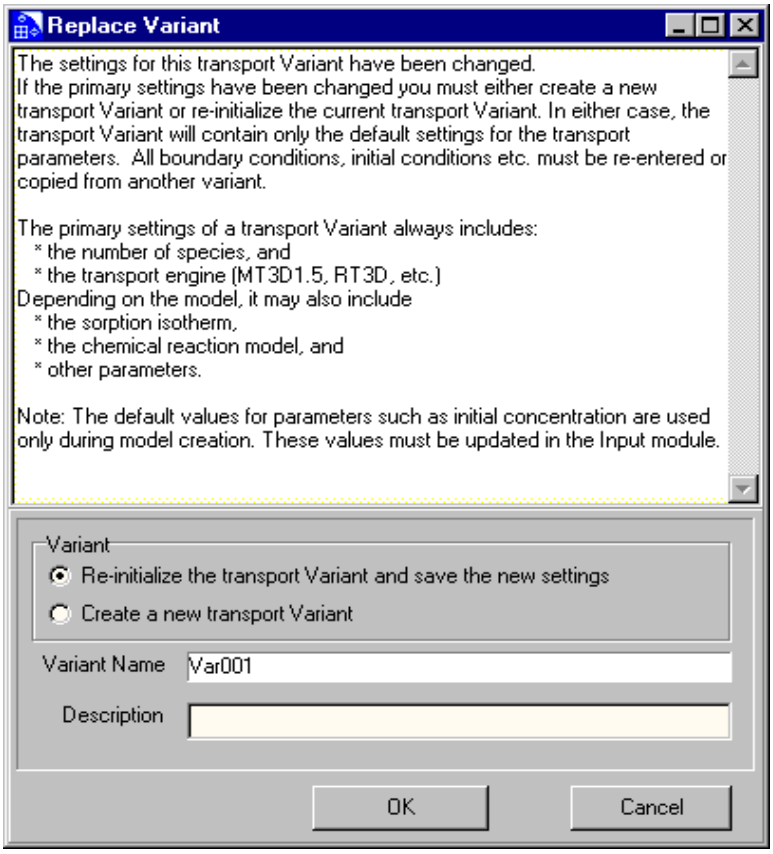

Transport Engine Options
Variant Name: Var001
Total number of species 4
Transport Engine: RT3D
Number of mobile species 3
Model Name: Double-Monod degradation model
Description:
Sorption (or dual-domain transfer)
Linear isotherm (equilibrium-controlled)
Reactions
Double-Monod degradation model
Species
General
Model Params
Species Params
Designation | Component Description | Mobile | SCONC([mg/L]) | SP1(1/[mg/L]) | ATOL | RTOL
eDonor | Electron Donor | yes | 0 | 0 | 0.0001 | 0.0001
eAcceptor | Electron Acceptor | yes | 0 | 0 | 0.0001 | 0.0001
Aqu. Bact | Aqueous phase mobile bacteria | yes | 0 | 0 | 0.0001 | 0.0001
Soil Bact | Soil-phase immobile bacteria | no | 0 | 0 | 0.0001 | 0.0001
New Species
Delete Species
Help
Ok
Cancel

The lower half of the **Transport Engine Options** window contains four data entry tabs used to define the initial transport parameter values for the selected Transport Variant. Most of the parameters defined in these tabs may be modified in the **Input/Properties** module of Visual MODFLOW, but the default parameter values should still be reviewed to ensure they are reasonable for the modeling objectives. The reference documentation for each of the numerical engines includes detailed descriptions of the parameters referenced on these tabs. The parameter names and descriptions have been chosen to make it easy to cross-reference parameters with the technical documentation. All the technical documentation can be found on the Visual MODFLOW Installation CD-ROM in an Adobe Acrobat .PDF file format.

Saving the Transport Variant

If a new Transport Variant is created, the setting will be automatically saved upon selecting [OK] in the Transport Engine Options window.

If changes are made to an existing Transport Variant, the following **Replace Variant** window will appear.


Replace Variant
The settings for this transport Variant have been changed.
If the primary settings have been changed you must either create a new transport Variant or re-initialize the current transport Variant. In either case, the transport Variant will contain only the default settings for the transport parameters. All boundary conditions, initial conditions etc. must be re-entered or copied from another variant.
The primary settings of a transport Variant always includes:
* the number of species, and
* the transport engine (MT3D1.5, RT3D, etc.)
Depending on the model, it may also include
* the sorption isotherm,
* the chemical reaction model, and
* other parameters.
Note: The default values for parameters such as initial concentration are used only during model creation. These values must be updated in the Input module.
Variant
Re-initialize the transport Variant and save the new settings
Create a new transport Variant
Variant Name
Var001
Description
OK
Cancel

The user will have two options:

- Re-initialize the transport variant and save the new settings
- Create a new Transport Variant

Re-initializing the Transport Variant

Re-initializing the Transport Variant will save all the changes made within the **Transport Engine Options** window to the same variant name. This will overwrite all of the information contained in the Variant file and reset the species specific transport properties and boundary conditions of the model.

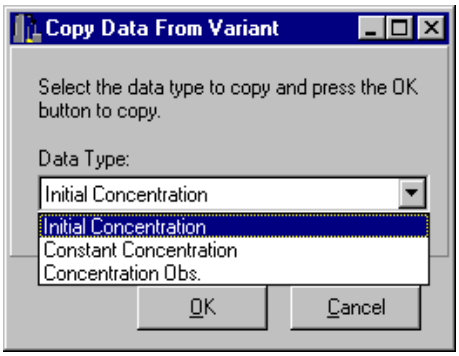
Creating a New Transport Variant

Creating a new Transport Variant will save and condense the old variant information to the Variant file (*project.var001*) and will then create a new Transport Variant and re-initialize the species specific transport properties and boundary conditions of the model.Regardless of which option is selected, the species specific information in the Input section will be re-initialized.

Copying a Variant

If changes are to be made to the Transport Engine, the Sorption method or the Reaction option, or if Species are added or deleted, then a new Transport Variant should be created. However, in this case it may be desirable to copy the initial concentrations, boundary conditions and observation data from one of the existing variants.

To copy model input data from an existing Transport Variant to the new Transport Variant select **Setup/Copy from Variant** from the top menu bar of the **Main Menu**. The following **Copy Data From Variant** window will appear:



Select the information to copy and then click **[OK]**. Depending on the data being copied, a second window will appear where the existing Transport Variant must be selected and the species from the existing Transport Variant must be mapped to the species in the new Transport Variant.

2.4 Entering the Model Data

When a new model is first created, it consists of a rectangular model domain with uniformly spaced grid cells, a uniform property values, and no boundary conditions. Naturally, this is simply a starting point to use for developing the 'real' model using the graphical tools provided in the **Input** section of Visual MODFLOW.

The **Input** section of Visual MODFLOW is used to define:

- refine the 3D finite difference grid,
- enter pumping well and observation well locations and attributes,
- define soil property zones and values,
- assign boundary condition locations and attributes, and
- define particle locations

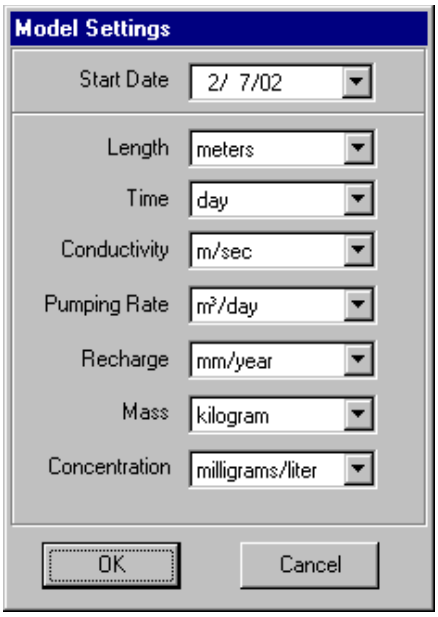
A detailed description of the graphical features and data manipulation tools available in **Input** section of Visual MODFLOW is provided in Chapter 3.

2.5 Changing Model Settings

Once the model has been created, it may be necessary to alter the units for one or more of the model input data types. The units for the model input data types may be changed from the **Main Menu** of Visual MODFLOW by selecting the **File/Change Units...** option. The following **Model Settings** window will appear.

The **Model Settings** window contains the simulation **Start Date** and unit picklists for each of the model input data types including:

- **Length**
- **Time**
- **Conductivity**
- **Pumping Rate**
- **Recharge**
- **Mass**
- **Concentration**



When modifying the units for selected data types, it is important to remember that Visual MODFLOW does **NOT** contain a unit conversion program. It will **NOT** transform the values already in the project to their equivalent values in the new system of units.

For example, if the length unit was in meters and it was changed to feet, any head values entered as 10 metres would now be read as 10 feet (i.e. they would not be altered to a value of 32.81 feet).

Therefore, if the units for any model data types are modified in the middle of developing the model it is strongly recommended that ALL model input parameters be carefully and thoroughly reviewed to ensure they ‘make sense’.

2.6 Overlay Control Options

Each different **Input**, **Run** and **Output** screen in Visual MODFLOW allows is used to assign, edit or display specific characteristics of the model. The display of the different model characteristics such as grid lines, property zones, boundary conditions and contour lines is organized as a series of separate “Overlays”.

Overlay Groups

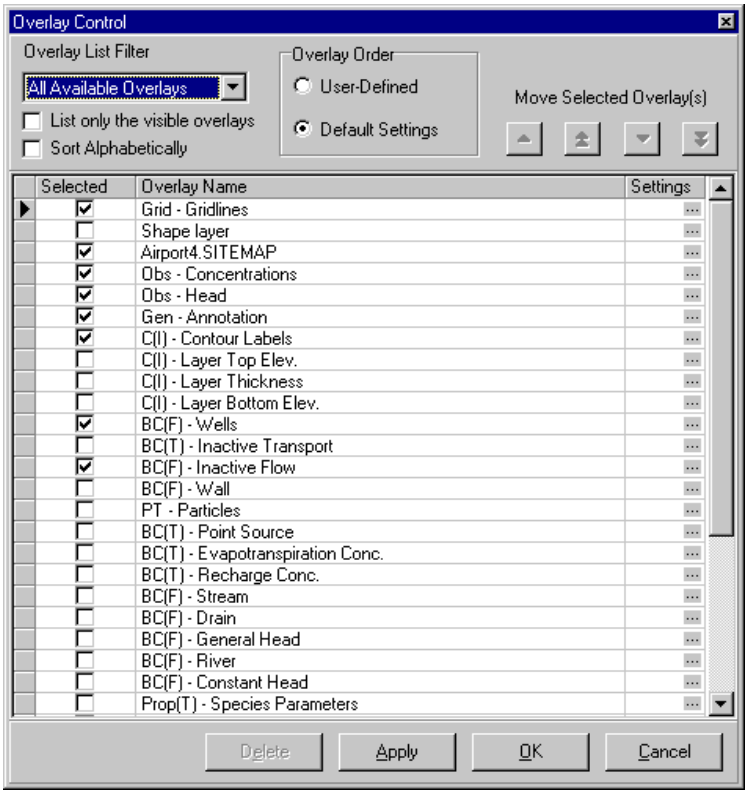
Due to the shear number of different Overlays available in Visual MODFLOW, the Overlays were divided into different groups to make it easier to manage the Overlay list. The Overlay Group Names and Short Names are as follows:

Group Name	Short Name	Description
Boundary Conditions	**BC(F)**	Flow boundary conditions
	BC(T)	Transport boundary conditions
Contours (Input)	**C(I)**	Contour maps of input parameters
Contours (Output)	**C(O)**	Contour maps of model output
General	**Gen**	General/miscellaneous overlays
Grid	**Grid**	Gridlines
Observations	**Obs**	Observation wells
Particle Tracking	**PT**	Particles and pathlines
Properties	**Prop(F)**	Flow properties
	Prop(T)	Transport properties
Sitemaps	**Map**	Site maps in .DXF or .BMP format

Note: The Overlays for the display of the modeling results (e.g. head contours, velocity vectors, pathlines) are only available in the **Output** section of Visual MODFLOW. Any Overlays related to the modeling results will not be available in the **Input** and **Run** sections.

Overlay Display Settings

The display status, display settings and view priority of each Overlay is controlled automatically by Visual MODFLOW using programmed (default) settings that turn selected Overlays on or off depending on which screen is currently active. However, the default Overlay settings can be customized using the **Overlay Control** by pressing the **[F9 - Overlay]** button in the bottom toolbar of the **Input**, **Run** or **Output** section. The following **Overlay Control** window will appear as shown in the following figure and described below.



Changing the Display Status of Selected Overlays

The Overlays currently being displayed are indicated by a checkmark in the **Selected** column. This display status (on or off) of each Overlay can be easily changed by clicking the checkbox to add or remove the checkmark.

In the Input section, the modified display status of each Overlay will be applied while viewing the current screen, but the default settings will over-ride these modifications when new **Input** module is selected.

In the Output section, the modified display status of each Overlay will be remembered the next time the model Output section is viewed.

Modifying the Display Settings of Selected Overlays

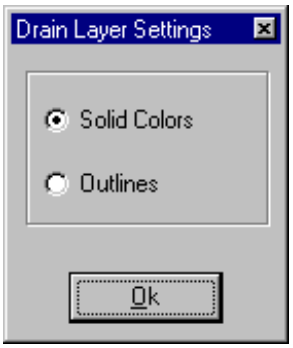
Most Overlays have different display settings controlling how they appear in the model. These options can be modified by clicking the **[...]** button under the **Settings** column of the **Overlay Control** window. Once the display settings are modified, the new settings are saved for all subsequent views.

The following is a description of the display settings for selected Overlay Group.

Boundary Condition and Properties Display Settings

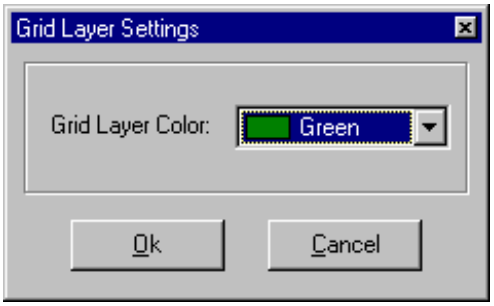
The display settings for the Boundary Conditions and Properties Overlay Groups has two options:

- **Solid Colors** displays the selected boundary condition grid cells using a solid color fill in each grid cell.
- **Outlines** displays an outline around the set of grid cells containing the selected boundary condition



Gridlines Display Settings

The display settings for the Gridlines may be used to change the color of the gridlines as shown in the following figure.



Contour Map Display Settings

The display settings window for Contour Maps is described in detail in the section Contour Maps on page 229.

Modifying the Overlay Order

The **Overlay Control** lists the Overlays in the order of their view priority, whereby the Overlay at the top of the list will be drawn overtop of the underlying Overlays. The **Overlay Control** has two options for defining the view priority of the **O**verlays;

(1) **User-Defined** where the view priority is customized by the user

(2) **Default** where the view priority is automatically set

In the **Input** section, the **Default** overlay order will likely be sufficient for the majority of cases, but in the **Output** section it will likely be necessary to manually adjust the overlays to achieve the desired presentation of results.

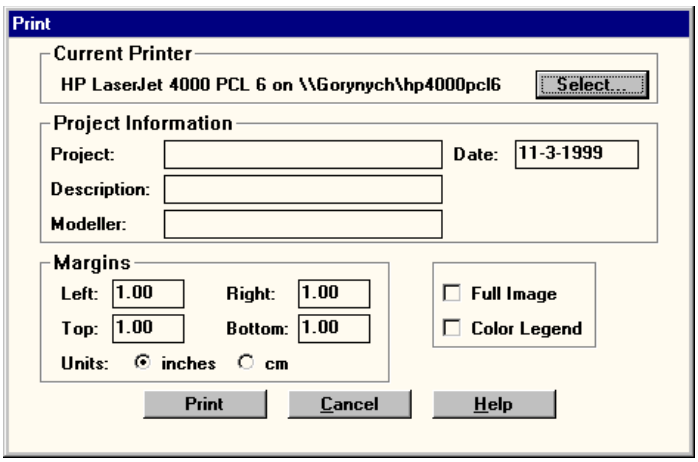
> **Note:** Visual MODFLOW will always remember the most recent Output Overlay display settings (i.e. each time the **Output** section is opened it will display the most recent **Output** Overlay settings).

The Overlay order can be modified by clicking the **User-Defined** option to activate the Up and Down Arrow buttons located below the Overlay List. Then select one (or more) Overlay and use the Arrow buttons move it up or down in the Overlay order.

Any modifications made to the Overlay order will be saved and applied when switching between different **Input** and **Output** screens.

2.7 Printing The Model Display Area

Visual MODFLOW will print the model display area currently being viewed in either the **Input**, **Run** or **Output** sections. To print the model display area select **File/Print** from the top menu bar the following **Print** window will appear.



Enter in the project information to provide the text for the title block. The Project, Description and Modeller fields will be included in the title blocks of the printed page unless the ☑ **Full Image** option is selected. If a Color Map is displayed, the **Color Legend** option may be used to show/hide the legend for the Color Map.

The default Windows printer is automatically selected as the current printing device. To change the current printer, click on the **[Select...]** button.

For details on printing a graph or bar chart, please refer to the Chapter 6 section Printing Options on page 280.

2.8 Export Options

Visual MODFLOW is able to export the model display area to several different graphics file formats and may also be used to export the modeling results to XYZ ASCII data files. The following sections provide describe the available Export options in Visual MODFLOW.

2.8.1 Exporting Graphics

As an alternative to printing the model display area to a printer, Visual MODFLOW can also export the model display area to a graphics file. Depending on the Overlay data set, the model display area may be exported to the following graphics file formats:

- AutoCAD (.DXF) - world or model co-ordinate system
- Enhanced Windows Metafile (.EMF)
- TecPlot ASCII (.DAT)* - world or model co-ordinates
- ESRI Shape (.SHP)** - world or model co-ordinates

* TecPlot ASCII (.DAT) is only available while viewing Output

** ESRI Shape (.SHP) is only available while viewing Output Contour Maps

To export the model display area to a graphics file,

- Select **File/Export...** from the top menu bar
- An **Export to file** window will appear
- Select the desired graphics **File type** and enter the **File name**
- Click the **[Save]** button

2.8.2 Exporting Data

The modeling results for a selected Output time can be exported to a tab-delimited ASCII data file for viewing or post-processing using a third-party graphics software package. To export the model results to a text file,

- Select **File/Export...** from the top menu bar
- An **Export to file** window will appear
- Select the **XYZ ASCII File type** and enter the **File name**
- Click the **[Save]** button

Contour data such as Head, Concentration, Drawdown, Water Table Elevation, etc. will be exported to an ASCII text file with the following format:

```
X     Y     Z     Value
```

Where;

`X` = X co-ordinate of the centre of the grid cell

`Y` = Y co-ordinate of the centre of the grid cell

`Z` = Z co-ordinate of the centre of the grid cell

`Value` = Contour data value for the grid cell

The grid cells are listed in order starting from the top left-hand corner of the bottom layer of the model and incrementing in the X-direction, then in the Y-direction, and then in the Z-direction.

3

Input Section - Assigning and Editing Data

This chapter presents information on:

- Building a new Visual MODFLOW model, and
- Editing an existing Visual MODFLOW model.

Visual MODFLOW stores all of the data for the flow, pathline and contaminant transport model in a set of files having formats and data structures which are quite different than the model input data files required by MODFLOW, MODPATH, and MT3D. There are many reasons for these differences, but the primary reasons are:

- Visual MODFLOW does not require consistent units for length and time. Instead, Visual MODFLOW allows mixed units for different model parameters (e.g. length in metres, pumping rate in US GPM, Recharge rate in mm/yr)
- Visual MODFLOW does not require boundary conditions to be defined in terms of stress periods. Instead, Visual MODFLOW allows each boundary conditions to be defined in using real time values and raw field data.

These differences are two of the key elements that make Visual MODFLOW so practical and user-friendly. However, these differences also require Visual MODFLOW to store the data in a different format and then translate these data files to the required format prior to running the models.

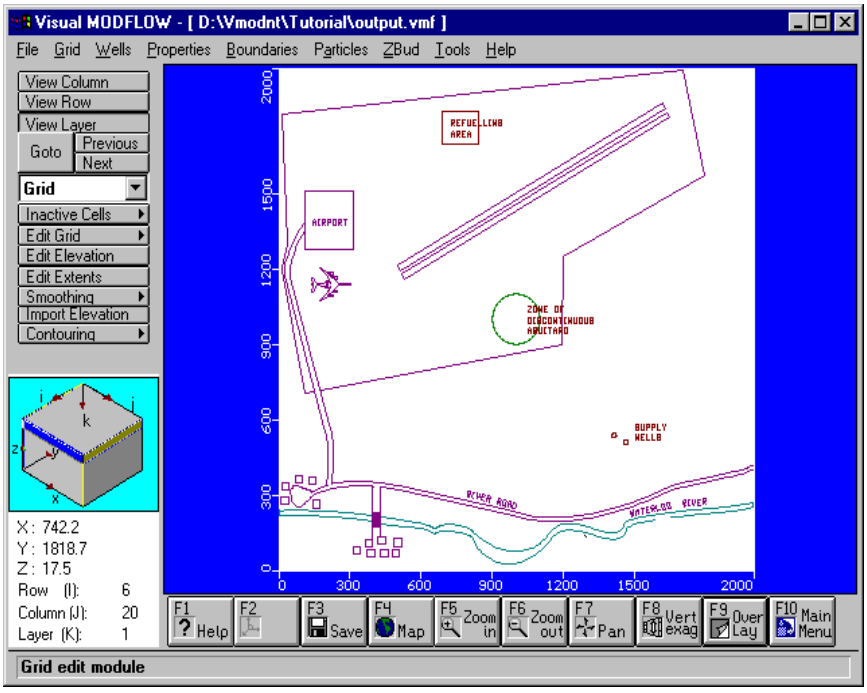
Most of input files are stored in ASCII text format (see Appendix A for details on the data formats for selected Visual MODFLOW input data files). As a result, the input files can be manipulated using a text editor or even generated using a FORTRAN or Visual Basic program, rather than using Visual MODFLOW's graphical user interface. However, if the files are externally manipulated or generated, the useful data validation and formatting checks performed by Visual MODFLOW will not be available. As a result, special care must be taken so the data structure for these files is not corrupted. **It is not recommended - other than in special situations - to externally edit or manipulate the data files using a text editor.**

The following sections provide detailed description of the features and functionality of the tools available in Visual MODFLOW for graphically building the model grid, assigning properties and boundary conditions, and defining particle locations and observation points.

General Input

To start a new Visual MODFLOW model follow the directions in Chapter 2 on creating a new model. To modify an existing Visual MODFLOW data set, click on **File/Open** in the **Main Menu** and select the desired Visual MODFLOW project (*projectname*.VMF) from the file window.

After opening an existing model or creating a new model, select **Input** from the **Main Menu**.



The **Input** section of Visual MODFLOW is used to define:

- the 3D finite difference grid,
- pumping well and observation well locations and attributes
- soil properties required for flow and contaminant transport
- boundary conditions for flow and contaminant transport
- particle locations for determining flow pathlines
- observation zones for determining flow and mass budgets

The top menu bar of the **[Input]** section contains menu items for the following:

File	Save the file, export, print or return to the **Main Menu**.
Grid	Create and modify the grid (This is the default screen when entering the **Input** section)
Wells	Insert, modify or delete pumping and observation wells
Properties	Add or modify hydraulic conductivities, storage properties, initial heads, initial concentrations, dispersion properties, and chemical reaction properties.
Boundaries	Input or modify flow and transport boundary conditions.
Particles	Insert or modify particle locations for particle tracking.
Zbud	Insert or modify zones used to calculate Zone Budget data.
Tools	Open the **Cell Inspector** to view cell-by-cell values, or open the **Annotation** screen to add lines, shapes and text in the model domain
Help	Obtain general help and version information.

3.1 File

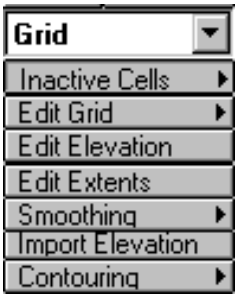
The **File** item in the top menu bar has the following menu options:

Save	Save the data set.
Export	Export the data to an ASCII file (world or local co-ordinates), a DXF file (world or local co-ordinates), or an EMF file.
Print	Print the screen to the current output device and select the printing device.
Main Menu	Return to the main screen.

3.2 Grid

The **Grid** module allows the user to define and discretize the modeling domain. The user can add or delete gridlines or remove cells from the computations.

When the **Grid** option is selected in the **Input** section, the tools along the left-hand menu bar will reflect grid specific options:



[Inactive Cells] Defines inactive zones (no flow cells) within the model domain.

[Edit Grid] Select from **Edit Rows**, **Edit Columns**, or **Edit Layers** to add, delete, move, refine or coarsen the model grid.

[Edit Elevations] View and modify the individual grid cell elevations.

[Edit Extents] Expand or contract the X and Y limits of the model grid.

[Smoothing] Smooth the grid spacing transition in the X and Y directions.

[Import Elevation] Import layer surface elevations from Surfer .GRD files or ASCII .TXT files.

[Contouring] Display the layer top elevations, layer thickness, and layer bottom elevations using contour lines.

Assigning Inactive/Active Regions

When the default model grid is initially created by Visual MODFLOW all grid cells are set as “active”, such that the model will try to calculate head values for each grid cell in the rectangular model domain. Unless otherwise specified by a boundary condition, the edges of the rectangular model domain will act as a no flow boundary.

However, in many situations the boundary conditions defining the edges of the model domain will not coincide with the exact rectangular shape of the model grid. In these situations the grid cells outside of the model boundaries may be designated as “inactive” or “no flow” cells. These inactive grid cells are ignored by the model and are not used in any of the calculations of flow, particle tracking or contaminant transport.

The inactive (or “no flow”) regions of the model are defined by selecting one of the **[Inactive cells >]** options from the left-hand toolbar.

Mark Poly. Active Digitize a polygon around a group of cells which will be designated as active. Left-click at the start point of the polygon to start digitizing the shape of the polygon and right-click near the start point to close the polygon.

Mark Inactive Digitize a polygon around a group of cells which will be designated as inactive (indicated by a solid green color). Left-click at the start point of the polygon to start digitizing the shape of the polygon and right-click near the start point to close the polygon.

Mark Single Designate grid cells as either active or inactive by clicking on individual grid cells, or by clicking-and-dragging across multiple grid cells. Click the left mouse button to designate cells as inactive, and click the right mouse button to designate cells as active.

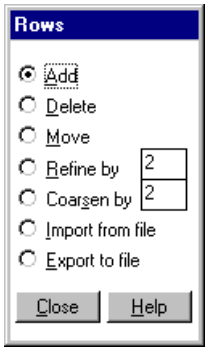
Copy Single Copy the active/inactive setting for individually selected grid cells to other layers/row/columns of the model.

Copy Polygon Copy the active/inactive setting for a group of grid cells defined by a polygon to other layers/rows/columns of the model.

Gridlines (Rows and Columns)

The maximum allowable dimensions of the grid are 500 grid lines (499 columns) in the X-direction by 500 grid lines (499 rows) in the Y-direction by 60 layers in the Z-direction. Thus, the maximum number of unknown hydraulic head values is 15,000,000. If these dimensions are insufficient for a specific problem please contact Waterloo Hydrogeologic for a customized version of Visual MODFLOW compiled specifically for the grid dimensions required.

When the default model grid is initially created by Visual MODFLOW, all of the grid cell have the same dimensions in the X, Y and Z directions. However, in many situations it is advantageous to have non-uniform grid spacing to allow for a finer grid discretization in the area of interest and larger grid spacing in areas which are less important, or where less data is available. The advantage of having a non-uniformly spaced grid is it allows the user get more detailed information in the area of interest while minimizing the number of grid cells used in the model. The reason for minimizing the grid size is to reduce the computational time required for each simulation.



To edit gridlines select **[Edit Grid >] Edit Columns** or **[Edit Grid >] Edit Rows** from the side toolbar. This opens a window with the following options:

Add Add individual gridlines by clicking the left mouse button at selected locations on the model grid. Use the right-mouse button to add a gridline at an exact location.

Delete Delete individual gridlines by clicking the left mouse button on selected gridlines.

Move Move individual gridlines by clicking the left mouse button on a gridline to select it, and then clicking the left mouse button again to place it at a new location.

Refine by Select a range of rows/columns between which each row/column will be subdivided into a specified number of rows/columns (e.g. **Refine by 2** would subdivide each row/column into two equally spaced rows/columns).

Coarsen by Select a range of rows/columns between which the number of gridlines will be reduced by a specified factor. (e.g. **Coarsen by 2** would reduce the number of rows/columns by a factor of 2).

Import from file Import gridline co-ordinates from a .TXT file. The format of the text file should be such that gridlines locations are in model co-ordinates and each gridline has a separate row.

Export to file Export the gridline co-ordinates to a .TXT file.

When adding a gridline, the new grid cells that are created take on the properties of the original cells that were sub-divided. Consequently, the parameter and elevation distribution remains the same when new cells are added.

When deleting a gridline, a single grid cell is created where there was once two or more grid cells. Consequently, the model properties and boundary conditions for the single grid cell is determined by the grid cell occupying the largest X-Y area prior to being deleted.

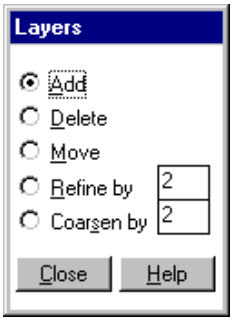
When a gridline is moved it is a combination of the **Delete** and **Add** option (i.e the line is first deleted from the original location and a new line is inserted at the new location). This can make it difficult to predict the resultant properties and boundary conditions for the revised model grid. To avoid these problems, if the model properties and boundary conditions have already been assigned, don't use the **Move** option, but rather **Add** a new gridline at the new location first and then **Delete** the old gridline.

Grid Layers

To modify layers, choose **[View Column]** or **[View Row]** and select a column or row in the model domain. This will "flip" the display from plan view to cross-section view.

To edit the model layers select **[Edit Grid >] Edit Layer** from the side toolbar. This opens a window with the following options:

> **Note: Edit Layer** options are ONLY available in cross-section view (**View Row** or **View Column**)



Add Add layer gridlines by clicking the left mouse button at selected locations on the model grid. Use the right-mouse button to add a layer gridline at an exact location.

Delete Delete layer gridlines by clicking the left mouse button on selected layer gridlines.

Move Move layer gridlines by clicking the left mouse button on a layer gridline to select it, and then clicking the left mouse button again to place it at a new location.

Refine by Select a range of layers between which each layer will be subdivided into a specified number of layers (e.g. **Refine by 2** would subdivide each layer into two equally spaced layers).

Coarsen by Select a range of layers between which the number of layer gridlines will be reduced by a specified factor. (e.g. **Coarsen by 2** would reduce the number of layers by a factor of 2).

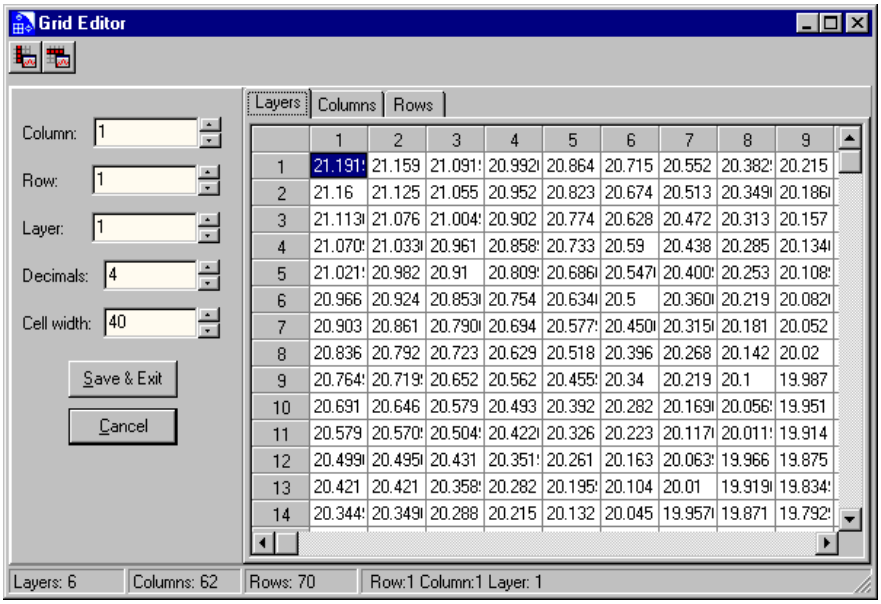
When adding a layer gridline, the new grid cells that are created take on the properties of the original cells that were sub-divided. Consequently, the parameter and elevation distribution remains the same when new cells are added.

When deleting a layer gridline, a single layer is created where there was once two or more layers. Consequently, the model properties and boundary conditions for the single layer is determined by the thickest grid cell prior to being deleted.

When a layer gridline is moved it is a combination of the **Delete** and **Add** option (i.e the line is first deleted from the original location and a new line is inserted at the new location). This can make it difficult to predict the resultant properties and boundary conditions for the revised model grid. To avoid these problems, if the model properties and boundary conditions have already been assigned, don't use the **Move** option, but rather **Add** a new gridline at the new location first and then **Delete** the old gridline.

Grid Cell Elevations

The individual grid cell elevations are usually defined by importing a data file containing measured values from the field and interpolating these values to each grid cell in a selected layer. However, in some circumstances, the imported data may not represent known elevation data for selected local locations. In these situations, the individual grid cell elevations need to be modified using the **[Edit Elevation]** option from the left-hand toolbar. The **[Edit Elevation]** option opens an **Edit Grid** window as shown in the following figure.



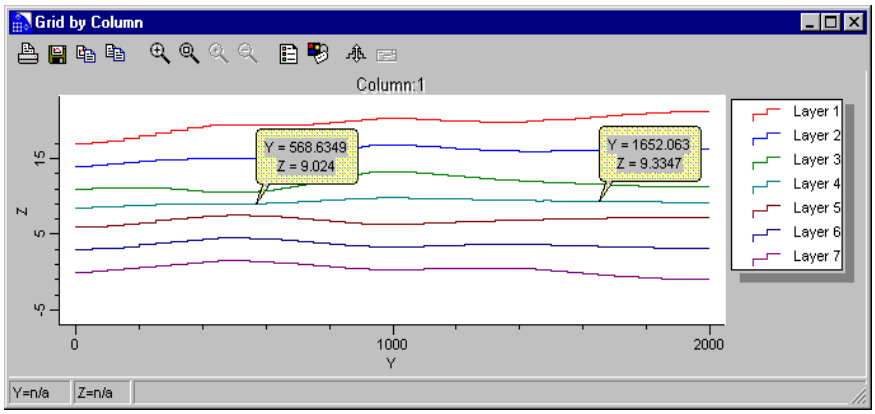
Along the top of the chart section of the grid editor, there are three tabs: **Layers**, **Columns**, and **Rows**. The grid elevation table displays the top elevation of the model grid cells corresponding to the I, J, K co-ordinates shown in the headers of the table.

- When viewing the **Layers** tab, the table displays the (I, J) grid co-ordinates
- When viewing the **Columns** tab, the table displays the (I, K) grid co-ordinates
- When viewing the **Rows** tab, the table displays the (J, K) grid co-ordinates

To quickly find a particular cell use the input boxes to the left of the grid. Simply enter the **Column**, **Row** and **Layer** coordinates of the cell and it will be highlighted in the table view.

Grid cell elevations can modified by entering new values directly into the cells of the table, or by moving selected grid lines up or down using the cross-sectional view of a selected column or row.

A cross-section of the grid for a selected row or column can be viewed by clicking the **[View by Column]** or **[View by Row]** icon in the top left corner of the **Edit Grid** window.



The **Grid by Column** or **Grid by Row** window displays a 2-D graphical representation of the column or row corresponding to the cell highlighted in the **Edit Grid** window. This cross-section view of the grid is displayed using the IChart component and can be viewed, printed, saved, exported, and modified as described in Chapter 6.

At any time move the cursor onto the graph, until a text bubble appears and click once with the left-hand mouse button to add a co-ordinate label.

The **[Edit Grid]** icon on the top toolbar can be used to select a gridline for an individual grid cell and drag it up or down to a new location.

The **[Save]** icon is used to apply any changes made to individual grid cell in the cross-section view to the elevation table spreadsheet in the **Grid Edit** window.

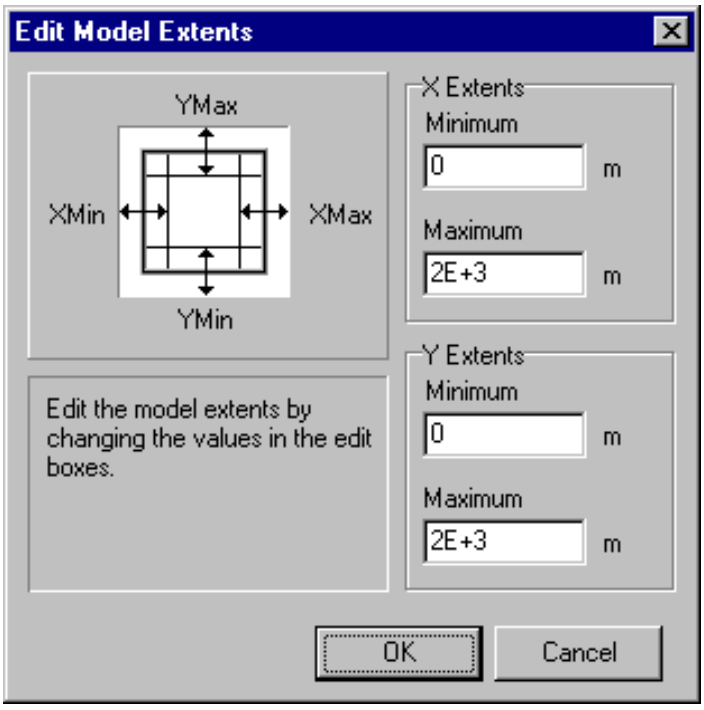
To return to the **Edit Grid** window press the close button **[X]** in the top right-hand corner of the **Grid by Column** or **Grid by Row** window.

To exit the **Grid Edit** window press the **[Save & Exit]** button to save any grid elevation changes, or press the **[Cancel]** button to cancel any changes.

Model Extents

As the model is being developed and calibrated and worked on, there may be situations when new information becomes available, or when the scope of the modeling project changes such that the dimensions of the model domain need to be modified (usually expanded to include regions outside the original model domain).

The horizontal extents of the model domain can be modified by select the **[Edit Extents]** option from the left-hand toolbar. The following **Edit Model Extents** window will appear.



The **Edit Model Extents** window is used to change the location of the outer most column or row gridlines.

The **X-Extents** indicate the **Minimum** and **Maximum** X-coordinate for the model domain.

The **Y-Extents** indicate the **Minimum** and **Maximum** Y-coordinate for the model domain.

The model domain can be enlarged by entering a lower **Minimum** value and/or a larger **Maximum** value for the **X-Extents** and **Y-Extents**.

The model domain can be decreased by entering a larger **Minimum** value and/or a smaller **Maximum** value for the **X-Extents** and **Y-Extents**.

> **Note:** The extents cannot be adjusted such that the outside row or column is less than 0.01 length units.

Click **[OK]** when all the values are entered. If the values are not valid a message box will appear stating the limits of the extents. The new model domain will span from the minimum locations entered to the maximum locations entered.

Grid Smoothing

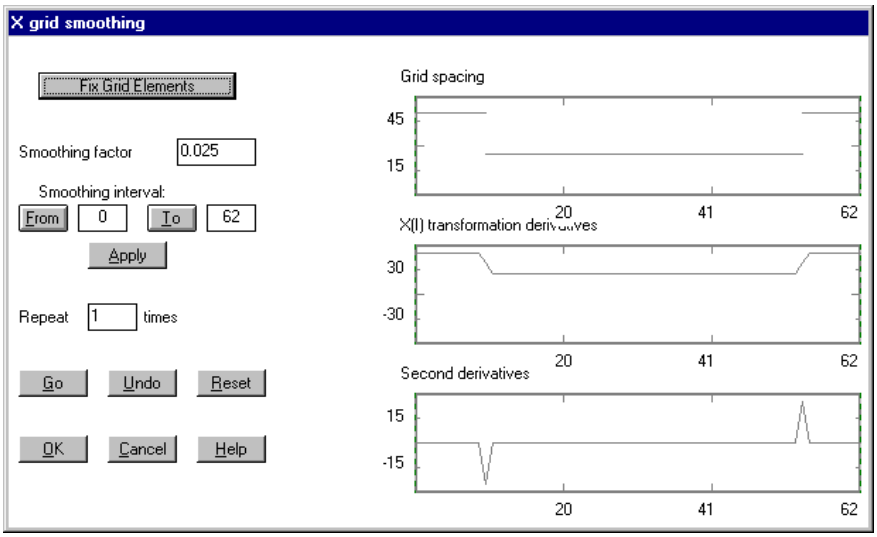
The computational efficiency of the MODFLOW solvers has been enhanced by the implementation of a grid-smoothing algorithm that optimizes discretization in non-uniform grids. Grid smoothing minimizes the possibility of poorly structured matrix equations, which can lead to convergence problems. An algorithm was developed by Waterloo Hydrogeologic Inc. to smooth a selected region of an arbitrary, non-uniform grid and then integrate the smoothed section back into the model without introducing additional irregularities into the grid. The smoothing algorithm was developed using a parabolic equation proportional to the second derivative of the grid spacing. Smoothing the grid discretization, by generating a new grid using a mathematical transformation of a uniform grid, creates a grid discretization that is no longer discontinuous. Grid smoothing maximizes the effectiveness of the grid and expedites complex grid discretization. Improvements to the accuracy of contaminant transport models have been achieved, as well as greater numerical stability and faster convergence for complex flow problems. The grid smoothing function facilitates minor grid improvements that may turn an oscillatory flow solution into a stable converging one.

A compromise must be reached between the accuracy of the model and the available computer resources when designing a finite-difference grid. Usually, only selected portions of the model domain, such as well fields, are refined, leaving the rest of the grid more coarsely discretized. In this case, stability is the trade-off; models that rely on a uniform grid are more stable and theoretically more accurate than non-uniform grids (Pinder and Gray, 1984). However, a sufficiently discretized uniform grid will result in extended simulation times.

A finer grid will normally give more precise results, especially in areas of steep hydraulic gradients. For best results, the grid spacing should change gradually. A rule of this is that the grid spacing should not increase by more than 50 percent between adjacent cells. Also an aspect ratio must be respected; a grid cell should not be more than 10 times bigger in one direction than in the other.

It is recommended that smoothing of the grid spacing take place before the adding model layers and boundary conditions because the calculation time required to modify a large grid is proportional to the number of layers.

To smooth the gridlines, select **[Smoothing >]** from the left-hand toolbar and then either **X smoothing** or **Y smoothing**. Depending on the selection, an X-grid smoothing window or a Y-grid smoothing window will appear as shown in the following figure.



Non-uniform grid spacing generally produces three typical patterns: sharp peaks, stairs, and isolated zigzags. A two-stage procedure is recommended for smoothing non-uniform grid spacing:

- Step (1): Intensive smoothing of small subintervals containing only one major change in spacing (smoothing factor equal or greater than 1).
- Step (2): Soft smoothing of the whole interval or large intervals containing smoothed subintervals from the first stage (with the smoothing factor much less than 1).

This method preserves regions of uniform spacing while providing smooth transitions in areas previously containing large changes in grid spacing. If only intensive smoothing is done all grid spacing will change whether it is necessary or not.

The following options are available in the window.

[Fix Grid Elements] Prevent single gridlines or gridline intervals from moving. (See Fixing Gridlines below).

Smoothing Factor Specify the smoothing intensity. The larger this parameter is, the more intensive the changes to grid spacing.

[From] Specify the left-hand boundary of the grid interval to be smoothed. Select this button and then click with the mouse on any graph to change the boundary. Alternately, enter the value in the **[From]** box using the keyboard.

[To] Specify the right-hand boundary of the grid interval to be smoothed. Select this button and then click with the mouse on any drawing to change the boundary. Alternately, enter the value in the **[To]** box using the keyboard.

[Apply]	Update changes to smoothing interval if changes were made directly to the **[From]** and **[To]** input boxes.
Repeat Times	Specify the number of smoothing repetitions to be performed after selecting **[Go]**.
[Go]	Start the smoothing procedure with the current settings.
[Undo]	Undo the last smoothing action, which includes repeats.
[Reset]	Restore the original grid before **[Go]** was first selected.

While in the window the grid spacing is only deformed interactively on the screen. Selecting **[OK]** permanently deforms the grid spacing and is irreversible unless you do not save all of your grid modifications upon leaving the grid menu.

Fixing Gridlines

In some regions of the grid, the grid spacing should not be adjusted during the grid smoothing process. For example, the grid spacing along a river boundary is set to reflect the river's width and should not be adjusted. The grid spacing can be fixed for designated grid intervals. By fixing a grid interval in place, you prevent the grid spacing from being adjusted during the smoothing process.

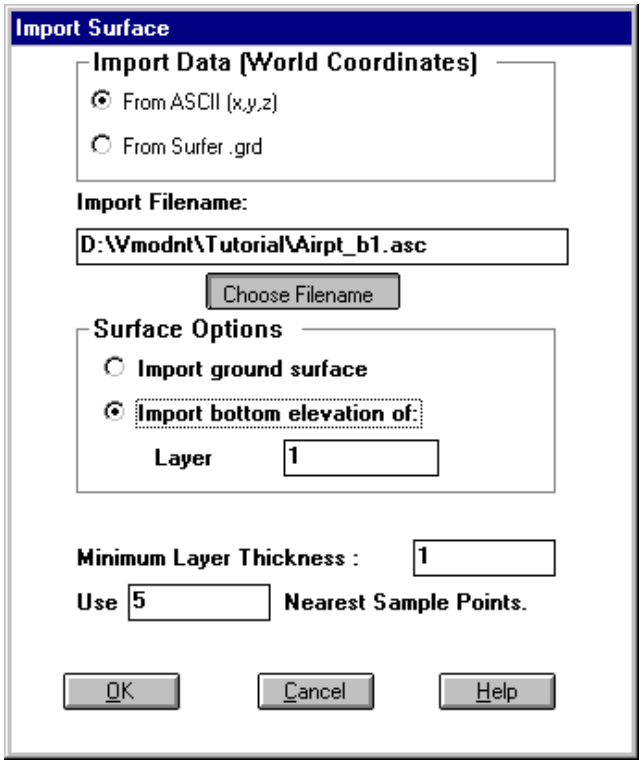
To fix gridlines, select **[Fix Grid Elements]**. The following menu selections will appear:

Fix Single	Fixes the location of a gridline that identifies a grid interval boundary. Left mouse button selects the gridline.
Release single	Releases a fixed gridline such that it no longer identifies a grid interval boundary. Left mouse button releases the gridline.
Fix interval	Selects a grid interval between two fixed gridlines within which the grid spacing will not be adjusted during the grid smoothing process. Left mouse button selects the grid interval. More than one grid interval may be selected.
Release interval	Releases a fixed grid interval. Left mouse button selects the grid interval to release.

Importing Surfaces

A numerical model using layers with constant elevations often cannot represent true hydrogeologic conditions caused by variable layer thickness and surface topography. In order to accommodate these conditions, Visual MODFLOW can import and interpolate external data files (Surfer™ .GRD or ASCII .TXT format) to create variable bottom and top elevations for each layer.

To import and interpolate data from an external file select the **[Import Surface]** option from the left-hand toolbar. The following **Import Surface** window will appear.



The **Import Data** frame is used to select the type of data file that will be imported.

- The **From ASCII (x,y,z)** option indicates the layer elevation data will be imported from an ASCII text file with three columns of data containing the X-coordinate, Y-coordinate and Z-elevation. This data file cannot contain any header information and each column of data must be space or comma separated.
- The **From Surfer .grd** option indicates the layer elevation data will be imported from a binary format Surfer™.GRD file created using a popular program named Surfer™ developed by Golden Software.

Note: The X-Y coordinates of the data points can be saved in either a model coordinate system or a world coordinate system.

The **Import Filename** field indicates the path and name of the data file being imported. The **[Choose Filename]** button is used to navigate to and select the data file and to select the X-Y coordinate system of the data being imported.

The **Surface Options** are used to select which layer surface is being imported:

- The **Import ground surface** option will import and interpolate the data for the top of Layer 1 (the upper most layer of the model).
- The **Import bottom elevation of:** option will import and interpolate the data for the bottom of the specified **Layer.**

The **Minimum layer thickness** defines the minimum distance between two adjacent layer surfaces. This minimum thickness overrides the interpolated elevation of a surface when two adjacent layer surfaces intersect. The top layer does not move and the imported layer will shift to accommodate the minimum layer thickness.

The **Number of nearest points** represents the number of nearest data points used to interpolate the elevation of the bottom or top of the grid cells using an inverse distance squared interpolation method. This changes the degree to which the surface is smoothed and the degree to which the interpolated surface represents the imported file.

The equation used for the interpolation is:

$$Z_{cell} = \frac{\sum_{i=1}^{n} \frac{Z_i}{d_i^2}}{\sum_{i=1}^{n} \frac{1}{d_i^2}}$$

Where:

Z_{cell} = elevation assigned to bottom of cell (or top of layer 1)

Z_i = elevation at a sample point

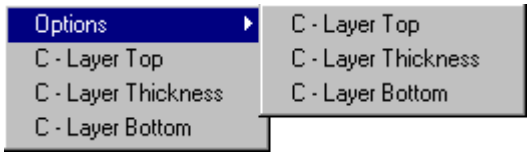
d_i = distance from the sample point to the cell centre; if $d_i = 0$ then $Z_{cell} = Z_i$

Contouring

The **[Contouring >]** button provides the option to display a contour map of:

- **Layer Top** elevations for the current layer
- **Layer Thickness** for the current layer
- **Layer Bottom** elevations for the current layer

The **Options** item provides access to the contour options for each of these **Contouring** overlays.



3.3 Wells

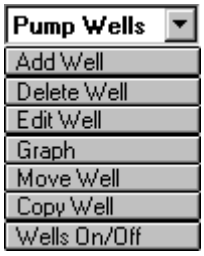
The **Wells** item in the top menu bar of the **Input** section is used to add, delete and edit three different types of wells:

- **Pumping Wells**
- **Head Observation Wells**
- **Conc. Observation Wells**

The features and functionality of the graphical tools available for each type of well are described in the following sections.

3.3.1 Pumping Wells

Pumping well data can be added to the model by selecting **Wells/Pumping Wells** from the top menu bar of the **Input** section. The **Pumping Wells** screen provides the following graphical options in the left-hand toolbar.



[Add Well] Adds a pumping well by clicking the mouse on the well location.

[Delete Well] Deletes a pumping well by clicking on the well.

[Edit Well] Edits the pumping schedule, screen location and grid co-ordinates of a selected pumping well by clicking on it.

[Graph] Displays a graph of pumping schedule vs. time for a selected pumping well by clicking on it.

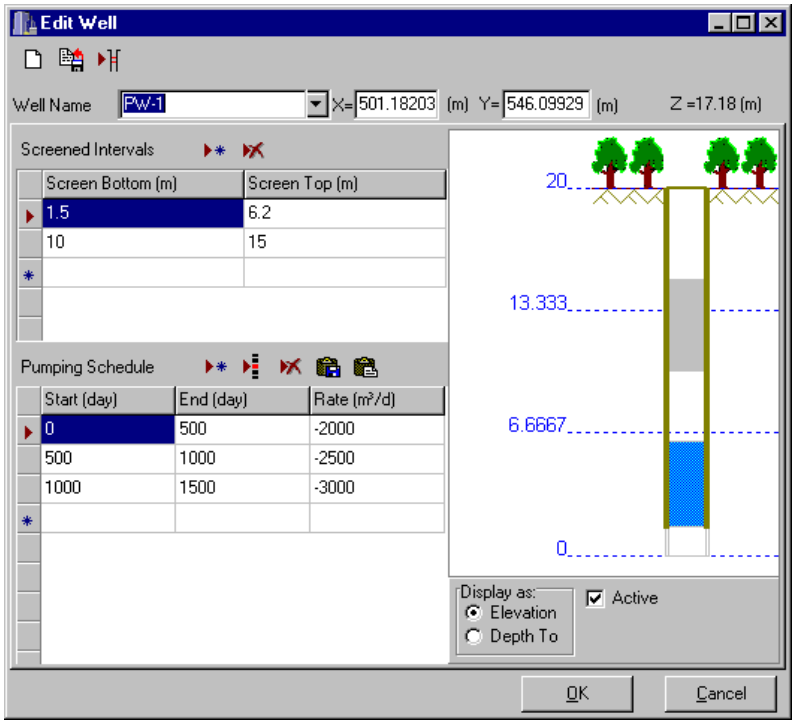
[Move Well] Moves a pumping well to a new location by clicking on it and then clicking on the new location.

[Copy Well] Copies a pumping well to different location by clicking on it to select it and then clicking on the different location(s) where it will be copied to. Since each pumping well requires a unique name, the default name of the new pumping well is the same as the original pumping well with a counter in brackets at the end of the name.

[Wells On/Off] Activates or deactivates a pumping well. Deactivated pumping wells will not be included in the simulation.

The number of pumping and injection wells is limited only by the amount of RAM available.

When the **[Add Well]** or **[Edit Well]** options are used, the **Edit Well** window will appear as shown in the following figure.



This window displays the relevant attributes of the pumping well including the **Well Name**, **X** and **Y** co-ordinates, **Screen Intervals**, **Pumping Schedule**, and the pumping well status (**Active/Inactive**). A diagram of the wellbore through the various model layers is displayed on the right-hand side of the window.

The **Display as:** option displays the vertical location of the wellbore in **Elevation** or **Depth** units.

The **Active** checkbox indicates whether the pumping well is active or inactive. If the Active checkbox is not selected, the pumping well will not be included in the simulation.

In the top left corner of the window, there are three icons as described below.

	[Clear]	Clears all screened intervals and pumping schedule information.
	[Reset]	Resets the pumping well information to the original settings prior to any changes being made.
	[Use as Obs.]	Allows the pumping/injection well to be used as head observation well. A second tab is added to the window for head observation information to be entered.

Well Name and Co-ordinates

The **Well Name** field requires an alphanumeric name used to identify the well and to label it on a map. This name must be unique and it may contain hyphens and spaces.

> **Hint:** When editing the pumping well data it is useful to remember that the **Well Name** field is a picklist. So instead of closing the **Edit Well** dialog and then clicking on another pumping well, use the **Well Name** picklist to select other pumping wells.

The **X** and **Y** fields contain the X and Y co-ordinates of the pumping well in the model co-ordinate system. If a new pumping well is added using the **[Add Well]** option the X and Y coordinates of the click location are automatically inserted in the **X** and **Y** fields. These values can be modified if data is available.

Visual MODFLOW maintains the X and Y co-ordinates independent of the model grid. Therefore, when the grid is modified the original pumping well location is not affected

> **Note:** MODFLOW considers a pumping well in a cell to be located at the centre of the grid cell and screened through the entire depth of the grid cell, regardless of the pumping well co-ordinates and well screen interval assigned in Visual MODFLOW. As such, a pumping well located in the corner of a grid cell will produce identical results as a pumping well located in the exact centre of the same grid cell.

Well Screen Intervals

Visual MODFLOW support pumping wells with multiple well screens throughout the length of the wellbore, and well screens that partially penetrate a model layer. However, it is important to note that MODFLOW does not have any special considerations for multiple well screens or grid cells containing partially penetrating well screens. As noted above, MODFLOW treats pumping wells as flux boundary conditions, such that each grid cell intersecting a well screen is assigned a specified flux. In a situation where a well is screen across several model layers, Visual MODFLOW uses the length of the well screen intersecting each model layer to determine the proportion of the total well pumping rate assigned to each well grid cell in the model. The following equation is used to calculate the pumping rate for each grid cell.

$$Q_i = \frac{L_i K_{xi}}{\sum (LK_x)_i} Q_T$$

Where,

Q_i is the discharge from layer i to a particular well in a given stress period,

Q_T is the well discharge in that stress period,

L_i is the screen length in layer i,

K_x is the hydraulic conductivity in the x-direction in layer i, and

$\Sigma(LK_x)_i$ represents the sum of the products of screen length and hydraulic conductivities in the x-direction of all layers penetrated by the well.

This approach, in which a multi-layer well is represented as a group of single layer wells, fails to take into account the inter-connection between various layers provided by the well. One of the most significant problems related to this approach is that well grid cells are essentially shut off when the water table is below the bottom of the grid cell. This automatically reduces the pumping rate of the well and may cause the water table to "rebound" and re-active the well grid cell. This type of on-again-off-again behavior for the pumping well(s) causes the solution to oscillate and may prevent the model from converging to a solution. In the event the model does converge to a solution, the model results may be misleading if one or more pumping wells having a lower than expected pumping rate.

Alternatively, a multi-layer well can sometimes be simulated by means of a vertical column of high permeability cells with a screen at the bottom of the column. Thus if the top part of the model becomes dry the total pumping rate is unaffected. This also takes into account the vertical inter-connection between layers. The downside of this approach is that the conductivity contrasts can lead to convergence problems.

Adding Well Screen Intervals

A well screen interval can be added graphically by right-clicking on the wellbore diagram and selecting the **Add Screen** option. Then click-and-drag the mouse from the start point of the well screen to the end point of the well screen.

The actual top and bottom elevations of each well screen interval are shown in the **Screened Intervals** table under the **Screen Top** and **Screen Bottom** columns, respectively. These values may be modified to more exact values if data is available.

Well screen data can also directly entered by clicking the **[Add Screen]** icon above the **Screened Intervals** table and entering the **Screen Bottom** and **Screen Top** elevations in the appropriate fields.

Each well screen interval requires data for the **Screen Bottom** elevation and the **Screen Top** elevation. If an additional well screen was accidentally added and does not contain any data for the **Screen Bottom** and/or **Screen Top**, this interval must be deleted from the **Screen Intervals** table before closing the **Edit Well** window.

Deleting Well Screens

Well screens can be deleted by either:

- Right-clicking on a well screen in the wellbore diagram and choosing the **Delete Screen** option,
- Selecting the well screen in the **Screened Intervals** table and clicking the **[Delete Screen]** icon above the table.

Well Pumping Schedule

The **Pumping Schedule** table is used to enter the well pumping rates for specified time periods. Negative pumping rate values are used for extraction wells, and positive pumping rates are used for injection wells.

Each time period requires a valid **Start** time, **End** time and pumping **Rate**. The **Start** time field is automatically generated to ensure that the time periods are continuous (i.e. **Start** time of one time period is equal to the **End** time of the previous time period). If the pumping schedule is not specified for the entire length of the transient simulation, then Visual MODFLOW will assume the well is shut off for the time where no information is available.

For steady-state simulations, the pumping rate for the first time period will be used as the steady-stage pumping rate.

Adding Pumping Schedule Items

To add an item to the **Pumping Schedule** table,

- Click the **[Append Schedule Item]** icon above the table to add a schedule item, or simply click in the first row of table.
- Enter an **End** time value and press the **<Tab>** key to advance to the **Rate** field
- Enter a pumping **Rate** value (remember to use a negative value for extraction wells)
- Press the **<Tab>** key again to create a new schedule item, or click the **[OK]** button to accept the pumping well data and close the **Edit Well** window

Each pumping schedule item is required to be completed with a valid **End** time and pumping **Rate**. If a pumping schedule item has been accidentally added without any data, it must be deleted before the **Edit Well** window can be closed.

Deleting Pumping Schedule Items

To delete an item from the **Pumping Schedule** table,

- Click on the item to delete in the **Pumping Schedule** table
- Click on the **[Delete Schedule Item]** icon above the table

Inserting a Pumping Schedule Item

To insert an item in the **Pumping Schedule** table,

- Click the time period where the new item will be inserted

- Click the **[Insert Schedule Item]** icon above the table
- Enter the **End** time for the new time period and press the **<Tab>** key to advance to the **Rate** column
- Enter the **Rate** value

Importing the Well Pumping Schedule

In situations where well pumping schedules have been recorded at regular intervals over a long period of time, the process of manually entering each schedule item can be tedious and time-consuming. For these situations Visual MODFLOW can import the well pumping schedule from an ASCII text file or from the Windows clipboard.

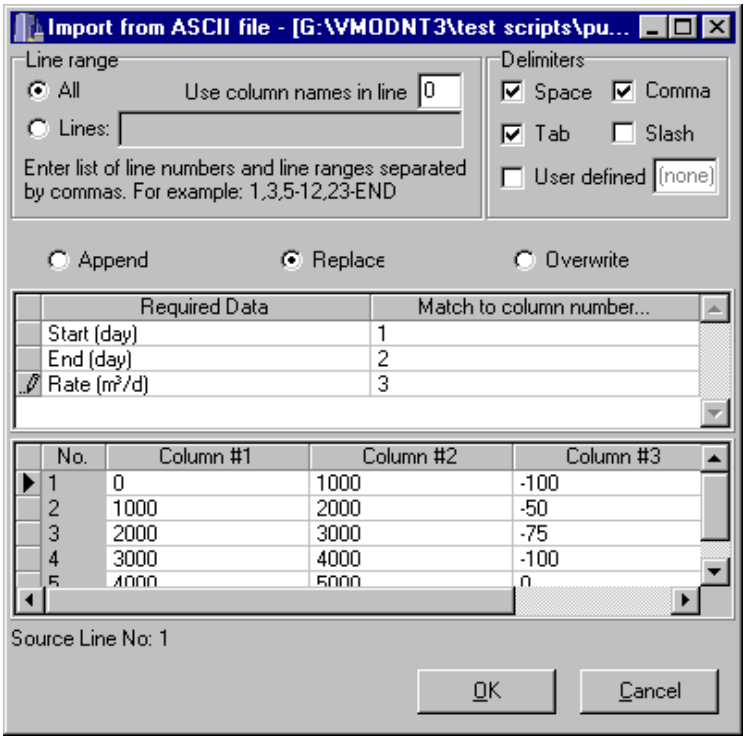
In either case, the data is required to be stored in the following format (see example below):

- At least three columns of data (**Start** time, **End** time and pumping **Rate**)
- Each schedule item must be stored in a different row
- The time periods must be continuous

```
Start Time     End Time      Pumping Rate
0              200           -500
200            400           -450
400            600           -350
600            800           -500
```

To import the schedule items from an ASCII text file click the **[Load Schedule Items from ASCII File]** icon and the **Import from ASCII file** window will appear as shown below.

To paste the schedule items into the **Pumping Schedule** table from the Windows clipboard click the **[Paste Schedule Items from Clipboard As Is]** icon and the **Import from Clipboard** window will appear. This option has the same functionality as the **Import from ASCII file** window described below.



The **Line range** frame provides the option of importing **All** lines of data from the well pumping schedule data file, or specifying a range of **Lines** to import from the data file.

The **Use column headers in line** field is used to identify which line of the data file contains the titles (header) for each column of data. The default setting is “0”, meaning no column headers are being used.

The **Delimiters** frame provides a selection of common delimiters used to separate different data values in the same row. If the required delimiter is not available in the pre-defined delimiters, a **User-defined** delimiter can be entered.

The **Append** option will append the imported data to the end of the current Pumping Schedule.

The **Replace** option will replace the current Pumping Schedule data with the imported data.

The **Match in column number** column is used to match the **Required Data** fields to the columns of data from the ASCII text file. In the figure above, the ASCII text file contained three columns of data; **Column #1** is matched to the **Start** field; **Column #2** is matched to the **End** field; and **Column #3** is matched to the **Rate** field.

When the **Start**, **End** and **Rate** fields are matched to the corresponding column from the source data, click the **[OK]** button to import the pumping schedule items.

Importing Pumping Well Locations

Although individual pumping wells may be easily added to the model using the **[Add Well]** option, this procedure may become tiresome and/or tedious for models containing several tens or even hundreds of pumping wells. In these situations Visual MODFLOW provides the option of importing pumping well locations, screen intervals and pumping schedules from an ASCII text file.

- Click on **File** from the top menu bar
- Select **Import** from the drop-down menu
- A **Import Wells** window will appear
- Select the data file
- Set the **Length units** and **Pumping Rate units** for the data file
- Click **[OK]** to import the pumping well data

The imported pumping well data file must be space delimited with no header line containing eight columns of data as described below.

```
Name   X   Y   Scrn#   ScrnTop   ScrnBot   Stop   Pump
```

Where:

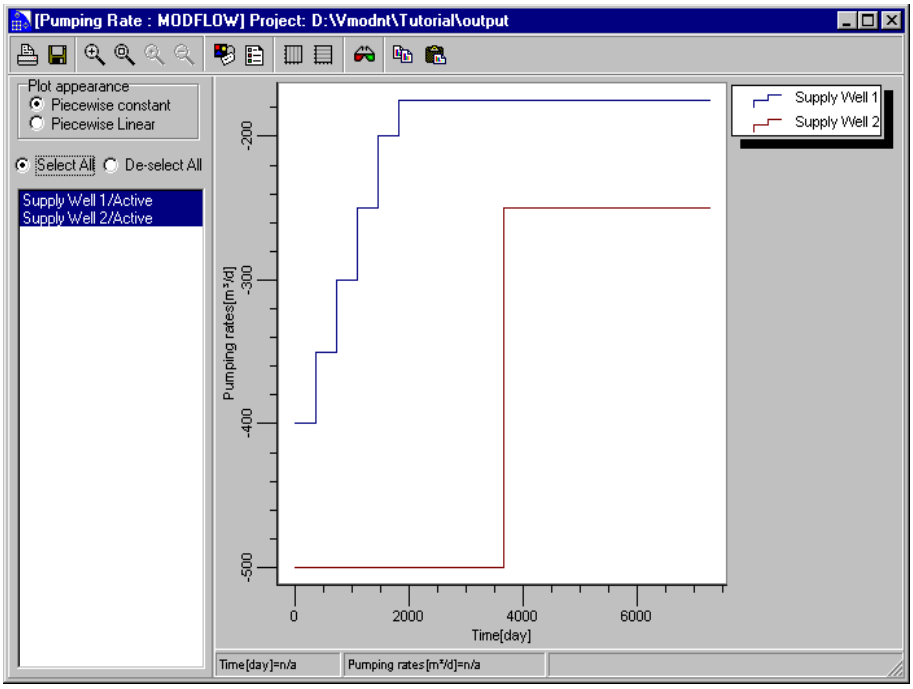
`Name`	= Well name
`X`	= Y co-ordinate
`Y`	= Y co-ordinate
`Scrn#`	= Screen ID number
`ScrnTop`	= Screen top elevation for each Screen ID
`ScrnBot`	= Screen bottom elevation for each Screen ID
`Stop`	= Stress period stop time (non-zero)
`Pump`	= Pump rate (-ve for discharge, +ve for injection)

For transient pumping schedules simply repeat the Name, X, Y Scrn#, ScrnTop and ScrnBot data for each time period.

Warning: Visual MODFLOW may act unpredictably when the co-ordinates are outside your model domain

Graphing Well Pumping Schedules

The **[Graph]** option will display a pumping rate vs. time graph for selected pumping wells. The following **Pumping Rate** graph window will appear. This graph is plotted using the IChart component described in Chapter 6.



The **Plot appearance** options control how the different pumping rate values are connected.

- The **Piecewise Constant** option plots the pumping rates as they are read by MODFLOW (i.e. constant for the duration of each time period with a sudden increase/descrease at the end of each time period).
- The **Piecewise Linear** option uses a single line to connect the pumping rates at the end of each time period.

Click the **Select All** option to view all of the pumping wells, click the **Deselect All** option to remove all pumping wells from the graph.

3.3.2 Head and Concentration Observation Wells

The Waterloo Hydrogeologic Inc. version of MODFLOW contains an enhancement designed to make model calibration more efficient. This Calibration Package saves the calculated heads at the locations of specified observation wells every time step in a .HVT file (Head versus Time). This allows the comparison of simulated heads with observed heads and produces calibration statistics and time series graphs at observation wells without saving the entire MODFLOW solution at every time step.

Head observation well data can be entered by selecting **Wells/ Head Observation Wells** from the top menu bar.

Concentration observation well data can be entered by selecting **Wells/ Conc. Observation Wells** from the top menu bar.

The following options appear along the left-hand toolbar:

[Add Obs.] Add an observation well.

[Delete Obs.] Delete an observation well.

[Edit Obs.] This feature allows you to edit the observation data associated with a selected observation well.

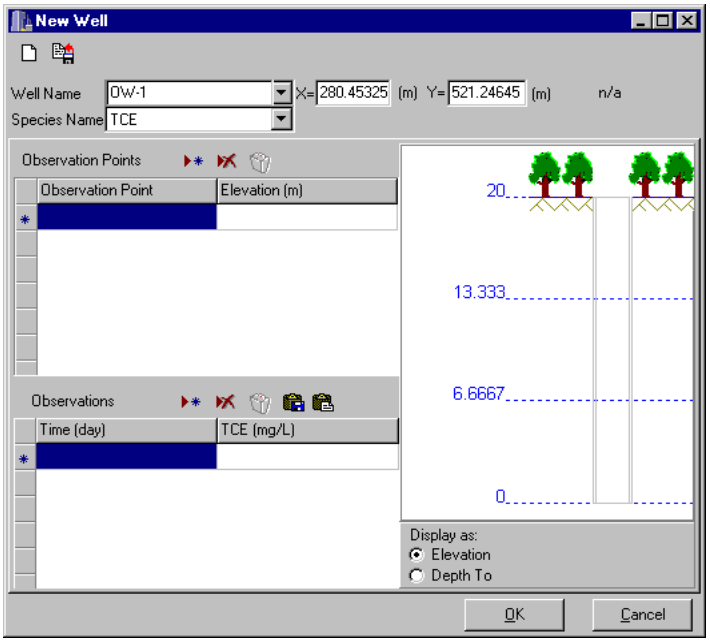
[Move Obs.] This feature allows you to move the observation well to a new position in the domain while maintaining the observation data.

[Import Obs.] Import observation well data. This feature allows you to import observation well data from a text file.

[Edit Groups] Create and edit groups of observation points to be used in the Run section and Output Module.

In cross-section, the observation wells are shown if they are contained within the specified row or column. A red line on the well identifies the location of the observation point. The plan-view locations of observation wells are indicated with a green marker.

If the **[Add Obs.]** or the **[Edit Obs.]** options are used to assign an observation well, a **New/Edit Well** window will appear as shown in the following figure and described below.



This window displays the relevant attributes of the observation well including the **Well Name**, **X** and **Y** co-ordinates, **Observation Points**, and **Observation Values**. A diagram of the wellbore through the various model layers is displayed on the right-hand side of the window.

The **Display as:** option displays the vertical location of the wellbore in **Elevation** or **Depth** units.

In the top left corner of the window, there are three icons as described below.

[Clear] Clears all observation points and observation values.

[Reset] Resets the head observation well information to the original settings prior to any changes being made.

The **Well Name** field requires an alphanumeric name used to identify the well and to label it on a map. This name must be unique and it may contain hyphens and spaces.

> **Hint:** When editing the observation well data it is useful to remember that the **Well Name** field is a picklist. So instead of closing the **Edit Well** window and then clicking on another head observation well, use the **Well Name** picklist to select other head observation wells.

The **X** and **Y** fields contain the X and Y co-ordinates of the observation well in the model co-ordinate system. If a new observation well is added using the **[Add Well]** option the X and Y coordinates of the click location are automatically inserted in the **X** and **Y** fields. These values can be modified if data is available.

Visual MODFLOW maintains the X and Y co-ordinates independent of the model grid. Therefore, when the grid is modified the original observation well location is not affected.

The **Species Name** field is present only for concentration observation wells. This field is a picklist used to select from the pre-defined list of dissolved species being simulated by the model.

Observation Points

The **Observation Points** are the elevations at which the **Observations** were recorded and/or collected. Although most monitoring or observation wells are installed with a well screen spanning a known interval of the aquifer, Visual MODFLOW requires a single observation point elevation to be defined instead of a well screen interval. The reason for using **Observation Points** as opposed to a well screen interval is because a well screen may span several vertical grid cells (layers) of the model and it would be impossible for Visual MODFLOW to “instinctively know” which grid cell to use for comparing observed values vs. calculated values. Therefore, a single observation point is used in order to eliminate any ambiguity regarding which model grid cell to use. However, for calibration purposes it is important to note that Visual MODFLOW simply compares the **Observations** for each observation point to the value calculated

in the grid cell where the observation point is located. Visual MODFLOW does not make any special adjustments to account for **Observation Points** which do not exactly correspond to the centre of the grid cell.

Visual MODFLOW supports head observation wells with multiple **Observation Points** throughout the length of the wellbore.

Adding Observation Points

An observation point can be added graphically by right-clicking on the wellbore diagram and selecting the **Add Observation Point** option. A horizontal line will appear in the wellbore diagram indicating the location of the observation point. Drag the observation point to the desired location within the wellbore.

The elevations of each observation point is shown in the **Observation Points** table. These values may be modified if data is available.

Observation point data can also directly entered by clicking the **[Add Observation Point]** icon above the **Observation Points** table and entering the **Elevation** value.

Each observation point requires data for the **Elevation**. If an additional observation point was accidentally added and does not contain any data for the **Elevation**, this observation point entry must be deleted from the table before closing the **Edit Well** window.

Deleting Observation Points

Observation Points can be deleted by either:

- Right-clicking on an observation point in the wellbore diagram and choosing the **Delete Observation Point** option,
- Selecting the observation point in the **Observation Points** table and clicking the **[Delete Observation Point]** icon above the table.

Observations

The **Observations** table is used to enter the observed values at specified times.

Each time period requires a valid **Start** time, **End** time and pumping **Rate**. The **Start** time field is automatically generated to ensure that the time periods are continuous (i.e. **Start** time of one time period is equal to the **End** time of the previous time period). If the pumping schedule is not specified for the entire length of the transient simulation, then Visual MODFLOW will assume the well is shut off for the time where no information is available.

For steady-state simulations, the observation for the first time will be used as the steady-stage observation.

Adding Observations

To add an item to the **Observations** table,

- Click the **[Add Observation Values]** icon above the table, or simply click in the first row of table.
- Enter an **Time** value and press the **<Tab>** key to advance to the **Value** field
- Enter an observation value
- Press the **<Tab>** key again to create a new schedule item, or click the **[OK]** button to accept the **Observations** data and close the **Edit Well** window

Each **Observations** table entry is required to be completed with a valid **Time** and observation value. If an **Observations** item has been accidentally added without any data, it must be deleted before the **Edit Well** window can be closed.

Deleting Observations

To delete an item from the **Observations** table,

- Click on the item to delete in the **Observations** table
- Click on the **[Delete Observation Value]** icon above the table

Importing Observations

In situations where observations have been recorded/collected at regular intervals over a long period of time, the process of manually entering each observation item can be tedious and time-consuming. In these situations Visual MODFLOW can import the observation data from an ASCII text file or from the Windows clipboard.

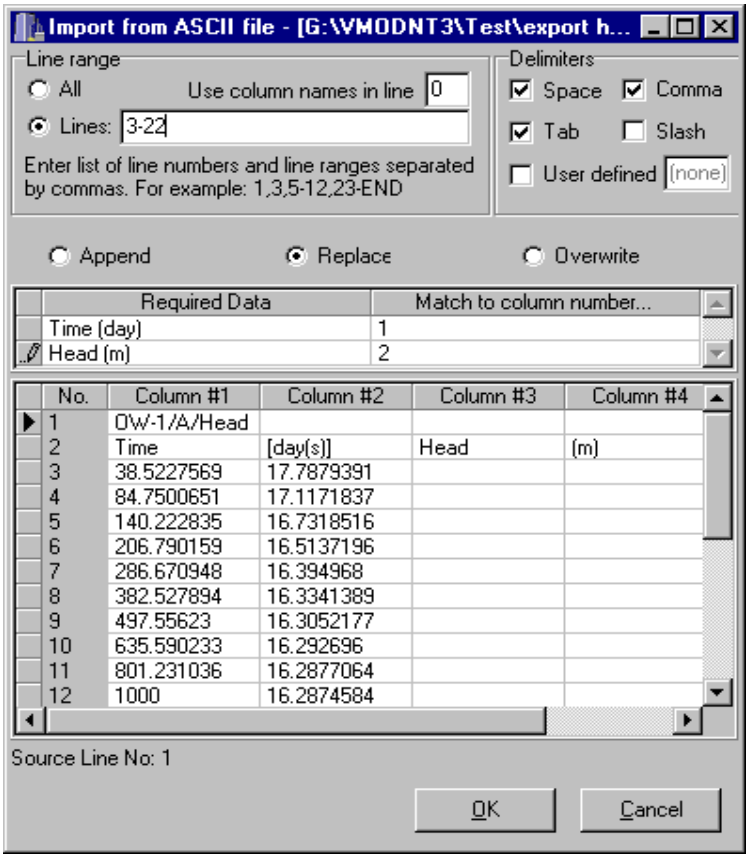
In either case, the data is required to be stored in the following format (see example below):

- At least two columns of data (**Time**, **Observation Value**)
- Each observation item must be stored in a different row
- The observation times must be sequential

```
Time            Observation
0               200.0
200             201.5
400             201.25
600             200.75
:
```

To import the schedule items from an ASCII text file click the **[Load Schedule Items from ASCII File]** icon and the **Import from ASCII file** window will appear as shown below.

To paste the schedule items into the **Pumping Schedule** table from the Windows clipboard click the **[Paste Schedule Items from Clipboard As Is]** icon and the **Import from Clipboard** window will appear. This option has the same functionality as the **Import from ASCII file** window described below.



The **Line range** frame provides the option of importing **All** lines of data from the well pumping schedule data file, or specifying a range of **Lines** to import from the data file.

The **Use column headers in line** field is used to identify which line of the data file contains the titles (header) for each column of data. The default setting is “0”, meaning no column headers are being used.

The **Delimiters** frame provides a selection of common delimiters used to separate different data values in the same row. If the required delimiter is not available in the pre-defined delimiters, a **User-defined** delimiter can be entered.

The **Append** option will append the imported data to the end of the current Pumping Schedule.

The **Replace** option will replace the current Pumping Schedule data with the imported data.

The **Match in column number** column is used to match the **Required Data** fields to the columns of data from the ASCII text file. In the figure above, the ASCII text file contained two columns of data; **Column #1** is matched to the **Time** field; and **Column #2** is matched to the **Head** field.

When the **Time**, and **Head** fields are matched to the corresponding column from the source data, click the **[OK]** button to import the pumping schedule items.

Importing Observation Well Locations

Although individual observation wells may be easily added to the model using the **[Add Obs.]** option, this procedure may become tiresome and/or tedious for models containing several tens or even hundreds of observation wells. In these situations Visual MODFLOW provides the option of importing observation well locations, observation points and observation values from an ASCII text file.

- Click the **[Import Obs.]** button from the left-hand toolbar
- An **Import Observations** window will appear
- Select the data file (data formats for these files are described below)
- Click **[OK]** to import the observation well data

Head Observation Wells

To import head observation well locations from a data file create a space-delimited (i.e. spaces as separators not commas) text file with the following format:

$Name_1\ X_1\ Y_1\ Z_1\ T_1\ H_1$

$Name_2\ X_2\ Y_2\ Z_2\ T_2\ H_2$

$Name_n\ X_n\ Y_n\ Z_n\ T_n\ H_n$

Where,

$Name_n$ = name of observation well (≤ 20 characters, no spaces)

X_n = X co-ordinate of observation well (world co-ordinate system)

Y_n = Y co-ordinate of observation well (world co-ordinate system)

Z_n = Elevation of observation point (i.e. elevation of screen)

T_n = Time of observation

H_n = Observed head

Each observed head must be on a new line. Observation well names and co-ordinates must be repeated if multiple observations are made for the same well.

Concentration Observation Wells

To import concentration observation well locations from a data file create a space-delimited (i.e. spaces as separators not commas) text file with the following format:

$Name_1$ X_1 Y_1 Z_1 T_1 $C_{001}...C_j$ $PtName_1$

$Name_2$ X_2 Y_2 Z_2 T_2 $C_{001}...C_j$ $PtName_2$

$Name_n$ X_n Y_n Z_n T_n $C_{001}...C_j$ $PtName_n$

Where,

$Name_n$ = Name of observation well (≤ 20 characters, no spaces)

X_n = X co-ordinate of observation well (world co-ordinate system)

Y_n = Y co-ordinate of observation well (world co-ordinate system)

Z_n = Elevation of observation point (i.e. elevation of screen)

T_n = Time of observation

$C_{001}...C_j$ = Observed concentration for j species of interest

$PtName$ = Optional observation point name

The order of the concentrations for a line of data must match the species order defined in your variant. Each observation time must be on a separate line. Therefore observation well names and co-ordinates must be repeated if multiple observations are made for the same well. If one or more of the species are not monitored during a particular sampling round, use a -1 to notify Visual MODFLOW that an observation does not exist. The following example shows a data file for a concentration observation well (OW1) with three species observed at three time intervals. The third species has no observations for the first two observation dates.

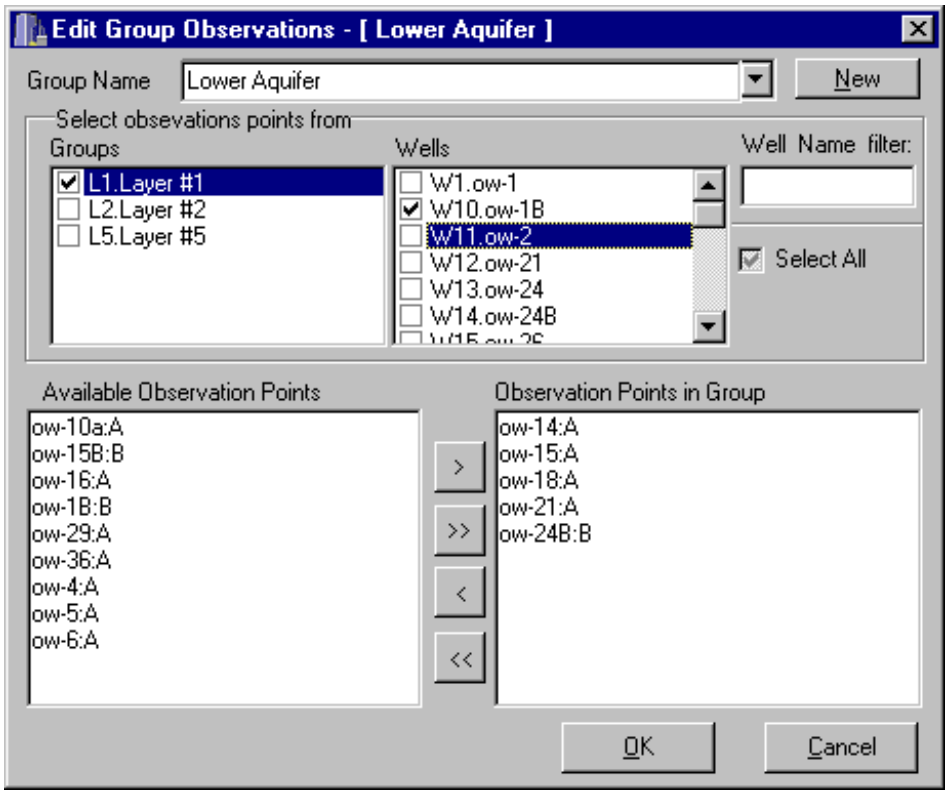
```
OW1 1000 1000 10 0 0 0 -1 A
OW1 1000 1000 10 365 550 50 -1 A
OW1 1000 1000 10 730 1100 100 10 A
```

Observation Groups

When the model is being calibrated using head and/or concentration observations, it is often very useful to be able to isolate and evaluate the quality of the calibration in

localized areas of the model, particularly in situations involving large regions and multiple aquifer units. For example, different Observations Groups may be created for the observation wells in each aquifer unit to easily evaluate the calibration in each aquifer. Additional Observation Groups may be created for on-site observations wells versus off-site observation wells, or observation wells may even be groups by quadrants such as North-East, North-West, South-East, and South-West. However, these are just a few examples of how the Observation Groups may be used.

The Observation Groups are assigned and edited in the **Input** section by clicking the **[Edit Groups]** button on the left-hand tool bar in the **Head Observation Wells** screen or the **Conc. Observation Wells** screen. The Edit Group Observations window will appear as shown in the following figure.



The **Edit Group Observations** window displays the Observation Points belonging to selected Observation Group. This window may be used to:

- Create a new Observation Group
- Add Observation Points to the selected Observation Group
- Remove Observation Points from the selected Observation Group

The **Group Name** field displays the name of the current Observation Group and contains a list of all available Observation Groups. A new Observation Group may be

created by pressing the **[New]** button and entering a description in the **Group Name** field.

The **Groups** list contains a list of all layers in the model containing Observation Points. Selecting one or more of these Layer Groups will add the associated Observation Points to the **Available Observation Points** list.

The **Wells** list contains a list of all Observation Wells in the model. When a well in this list is selected the Observation Points associated with the selected well are added to the **Available Observation Points** list.

Once all of the desired Observation Points are included in the list of **Available Observation Points**, use the arrow buttons to add/remove individual Observation Points to/from the list of **Observation Points in Group**.

3.4 Properties

A groundwater flow and contaminant transport model requires many different types of data to simulate the hydrogeological and hydrogeochemical processes influencing the flow of groundwater and migration of dissolved solutes. In Visual MODFLOW the hydrogeological and hydrogeochemical characteristics of the model are classified into the following input properties:

- Conductivity (K_x, K_y, K_z)
- Storage (S_s, S_y, P_{eff}, P_{tot})
- Initial Heads
- Bulk Density
- Model Params. (Stoichiometry)
- Species Params. (K_d, Decay)
- Initial Concentrations
- Dispersion (D_l, D_t, D_v, Diffusion)

As noted in the list above, some of these model properties require data for several different parameters (e.g. Conductivity requires values for K_x, K_y, and K_z). These model properties, and the associated set of parameters, are assigned using different input screens for each property. The active **Properties** screen will always be displayed in the **Current Overlay** field on the side menu bar.

A flow model requires Conductivity, Storage and Initial Heads property values for each active grid cell in order to run the flow simulation. Upon entering the **Conductivity** or **Storage** input screens, Visual MODFLOW will prompt for default property values for K_x, K_y, K_z, S_s, S_y, P_{eff}, and P_{tot}. The default values entered here will be assigned to every cell in the model domain. This will ensure the model has the minimum data required to run a flow model.

In most situations, the model properties will not be uniform throughout the entire model domain and it will be necessary to assign different property values to different areas of

the model. Heterogeneous model property values are supported by Visual MODFLOW using either Constant Value Property Zones, or Distributed Value Property Zones. These two different approaches are described below.

Constant Value Property Zones

The Constant Value Property Zones approach is the most simple and straight forward and can be used for all model properties supported by Visual MODFLOW. Different model properties are accommodated by grouping grid cells sharing the same property values into “property zones”. Each property zone may contain a unique set of property values and is represented by a different grid cell color.

The Constant Value Property Zones approach requires the development of a conceptual model, whereby each hydrostratigraphic unit of the model is assigned a uniform set of property values. For example, consider an aquifer where there is pumping test data and slug test data indicating a range of horizontal conductivity values from $1x10^{-4}$ cm/s to $5x10^{-4}$ cm/s at different locations within the aquifer. The conceptual approach would assign a uniform K_x and K_y value of $2.5x10^{-4}$ cm/s to the entire aquifer. This value would be adjusted up or down for calibration purposes within the range of values reported. If a reasonable calibration cannot be achieved using this conceptual model, it may be necessary to sub-divide this region into several zones to accommodate local irregularities in the flow pattern. However, almost all modeling textbooks strongly recommend to start out simple first and get as close as possible, and then make the model more complex only if necessary.

Distributed Value Property Zones

The Distributed Value Property Zones approach is currently only available for Conductivity and Storage properties. This approach is a little more complicated because it involves linking a property zone to one or more parameter distribution arrays containing data interpolated from scattered observation points. When a property zone is linked to distribution array, the property values assigned to each grid cell within that zone are calculated by multiplying the zone parameter value with the corresponding value from the parameter distribution array. If the grid spacing from the model does not match the grid spacing from the distribution array, a bivariate interpolation scheme is used to calculate the appropriate parameter value at the center of the model grid cell using the four nearest data nodes in the parameter distribution array.

For example, consider a model with 5 rows, 5 columns, 1 layer and 3 different Conductivity zones. The attributes of each conductivity zone are described in the following table:

Table 3.1				
	Zone Parameter Values			Linked to
Zone #	Kx (cm/s)	Ky (cm/s)	Kz (cm/s)	Distribution Array
1	0.001	0.001	0.0001	No
2	0.005	0.005	0.005	No
3	1	1	1	Yes

The arrangement of Conductivity property zones on the model grid is described in Table 3.2a, the Kx Distribution Array is described in Table 3.2b, and the resultant Kx values are shown in Table 3.2c.

Table 3.2a: Conductivity Zones On The Model Grid

		Columns				
		1	2	3	4	5
	1	1	1	1	2	3
	2	1	1	2	3	3
Rows	3	1	2	2	3	3
	4	2	2	3	3	3
	5	2	2	3	3	3

Table 3.2b: Interpolated Kx Values from a 5x5 Distribution Array

		Columns				
		1	2	3	4	5
	1	0.0011	0.0012	0.0014	0.0016	0.0019
	2	0.0013	0.0014	0.0016	0.0017	0.0021
Rows	3	0.0015	0.0016	0.0018	0.0018	0.0022
	4	0.0012	0.0013	0.0019	0.0021	0.0025
	5	0.0011	0.0011	0.0015	0.0019	0.0021

Table 3.2c: Model Kx Values

		Columns				
		1	2	3	4	5
	1	0.001	0.001	0.001	0.005	0.0019
	2	0.001	0.001	0.005	0.0017	0.0021
Rows	3	0.001	0.005	0.005	0.0018	0.0022
	4	0.005	0.005	0.0019	0.0021	0.0025
	5	0.005	0.005	0.0015	0.0019	0.0021

In Table 3.1 only Property Zone #3 is linked to a distribution array. Therefore, only the model grid cells containing property zone #3 are calculated using the Kx distribution array. The grid cells containing Property Zone #1 and #2 retain the Kx values specified for each zone.

As shown in the above example, both Constant Property Value Zones and Distributed Property Value Zones can co-exist in the same model, and in the same layer, such that some zones contain constant values and other zones contain distributed values interpolated from external data points.

When the Distributed Property Value Zones are initially imported into Visual MODFLOW they are each assigned zone parameter values of 1.0. This zone parameter value is used as a multiplier for modifying the distributed property values within this zone during the model calibration process.

3.4.1 Tools for Assigning and Editing Properties

The different property zones are assigned and modified in Visual MODFLOW using an assortment of graphical tools appearing on the side menu bar of each Properties screen.

[Import] Import and interpolate property data from discrete data points (currently only available for Conductivities, Storage and Initial Heads).

[Assign] Assign a selected property zone to a **Single grid** cell, a **Line** of grid cells, a **Polygon** of grid cells, or a rectangular **Window** of grid cells (see description on page 85).

[Edit] Edit the property zone assigned to a **Single** cell, or edit the parameter values for a selected **Property** zone (see description on page 86).

[Copy] Copy a **Single** property zone from a selected grid cell to other grid cells, or copy all property zones from the current **Layer/ Column/Row** one or more model layers/columns/rows (see description on page 87).

[Database] View and edit the property database.

[Contouring] View contour maps and/or color maps of the property value distributions and modify the contour map and color appearance **Options**.

Each of these tools are described in the following sections.

Importing Distributed Property Data

Visual MODFLOW v.3.0 now has a built-in Property Data Import Wizard to import and interpolate model property values (Conductivities, Storage and Initial Heads) from discrete data points using a selection of three popular data interpolation schemes including:

- Inverse distance squared
- Kriging
- Natural Neighbor

The data file formats currently supported by Visual MODFLOW for importing and interpolating model property data include:

- ASCII text files (.TXT)
- Excel spreadsheets (.XLS)
- GIS shape files (.SHP, point and line formats only)

The Property Data Import Wizard generates a distribution of model property values for either an entire layer(s) of the model, or within a specified region of the model defined by an existing model property zone(s).

When a data file is interpolated using the Property Data Import Wizard, Visual MODFLOW creates a distribution array for each of the required property parameters (e.g. Conductivity requires separate distribution arrays for K_x, K_y and K_z). Each distribution array consists of a two-dimensional grid of data with uniform spacing in the X and Y directions. These distribution arrays are “linked” to selected property zones within the model. If a property zone is linked to a distribution array, the parameter value for each grid cell in this zone is calculated by multiplying the parameter value for this zone by the corresponding interpolated value from the distribution array. When the model grid spacing does not correspond to the grid dimension of the distribution array, a bivariate interpolation scheme is used to calculate the property value for each model grid cell.

The Data Import Wizard involves the following five steps:

- Step 1: File Selection (see description below)
- Step 2: Matching Fields (see description on page 74)
- Step 3: Data Validation (see description on page 76)
- Step 4: Interpolation Options (see description on page 77)
- Step 5: Create/Select Property Zones (see description on page 82/85)

To import and interpolate a set of data for a model property, click the **[Import]** button on the left-hand menu bar of each property module screen to start the five step Property Data Import Wizard. Each of the five steps is described below using an example of importing data for Conductivity.

Step 1: File Selection

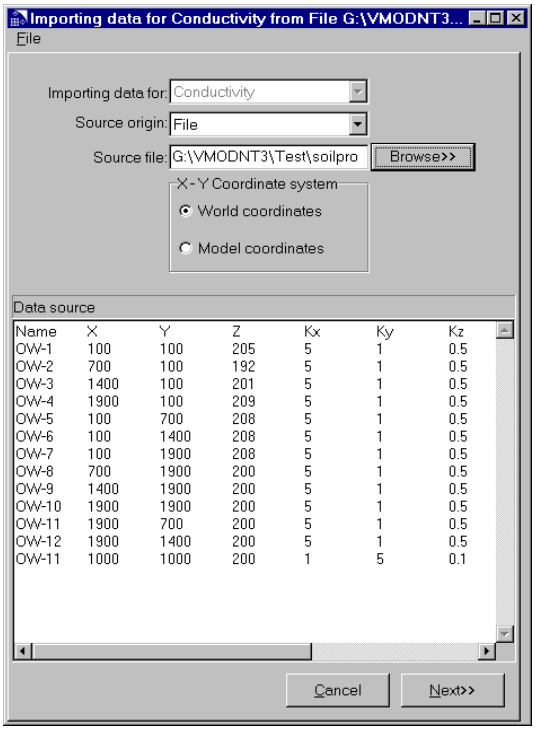
The first step of the Property Data Import Wizard is selecting the source data file. As mentioned above, Property Data Import Wizard supports three different data formats including ASCII test files, Excel spreadsheets, and GIS shape files (points and lines). If the source data is stored in a different format, but is in a tabular format, it can also be copied-and-pasted from the Windows clipboard.

The figure below is a screen capture of the first screen of the Property Data Import Wizard followed by descriptions of the fields and functionality of this screen.

Importing data for: indicates the model property data type. This field is determined by the active Properties screen in Visual MODFLOW and can not be modified.

Source origin: indicates whether the data is being read from a data file or from the Windows Clipboard. The default setting is to read the data from a file.

Source file: indicates the name of the source data file being imported. Use the **[Browse]** button to select the file type (.TXT, .XLS, or .SHP) and navigate to the location of the source data file. If the data is being copied from the Windows clipboard, the **Source file:** field is disabled and the **[Browse]** button becomes a **[Load]** button to load the data from the Windows clipboard.


Importing data for Conductivity from File G:\VMODNT3...
File
Importing data for: Conductivity
Source origin: File
Source file: G:\VMODNT3\Test\soilpro
Browse>>
X-Y Coordinate system
World coordinates
Model coordinates
Data source
Name X Y Z Kx Ky Kz
OW-1 100 100 205 5 1 0.5
OW-2 700 100 192 5 1 0.5
OW-3 1400 100 201 5 1 0.5
OW-4 1900 100 209 5 1 0.5
OW-5 100 700 208 5 1 0.5
OW-6 100 1400 208 5 1 0.5
OW-7 100 1900 208 5 1 0.5
OW-8 700 1900 200 5 1 0.5
OW-9 1400 1900 200 5 1 0.5
OW-10 1900 1900 200 5 1 0.5
OW-11 1900 700 200 5 1 0.5
OW-12 1900 1400 200 5 1 0.5
OW-11 1000 1000 200 1 5 0.1
Cancel
Next>>

The **X-Y Coordinate system** indicates the coordinate system of the data points being imported. **World coordinates** are typically referenced to a standard national or regional coordinate system **such as UTM, while** Model coordinates are referenced to the X-Y coordinate system of the model grid. The default setting is World coordinates.

The **Data source** panel displays a preview of the source data file being used to generate a distribution of property values.

Once a data set has been selected, press the **[Next]** button to advance to the next step.

Step 2: Match Fields

The second step of the Property Data Import Wizard involves matching the columns from the source data file to the data fields required by Visual MODFLOW to import

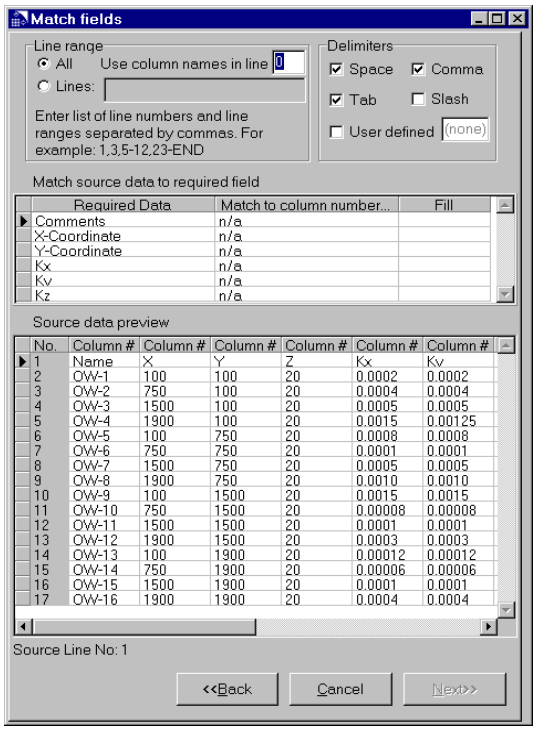
and interpolate the selected property values. A screen capture of the **Match fields** window is shown in the figure below.

Line range frame

The **Line range** frame is used to specify the line numbers to import from the data source.

The **All** option will use every line of data in the data file.

The **Lines** option will import only the data from the specified lines (rows) of data. An example of the format required to define the ranges of lines is provided in the space below the **Lines** field.



The **Delimiters** frame is used to identify the character string used as a separator for each column of data. The appropriate delimiter must be selected in order to properly parse the data file and obtain the correct values. When the correct delimiter is selected, the **Source data preview** table at the bottom of the window will display each field in separate columns.

The **Required fields** column lists the fields that need to be matched to a column of data from the source file. For Conductivities and Storage, the **Required fields** column includes several different parameter fields because each property zone requires data for multiple parameters (e.g. each Conductivity property zone requires values for **Kx**, **Ky** and **Kz**). The **Comments** field is optional (does not need to be matched to a column of data) because it is typically used for storing the Station ID (or "well name") information.

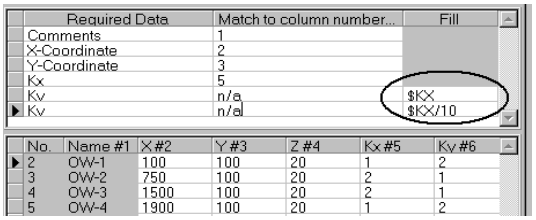
The **Match to column number…** column is used to identify the column numbers from the source file corresponding to each required field. If a data source does not contain values for each of the required fields, the unmatched fields may be left either blank or as "**n/a**" ("not applicable") and a fill value or expression may be entered.

The **Fill** column is used to define a constant value for the required parameter(s), or to define formulas to calculate the values for the required parameter(s).

As a minimum requirement, the **X-Coordinate**, **Y-Coordinate** and one parameter need to be matched to a column of data from the source file. If the source file does not contain data for all of the required parameters, the **Match to column number...** value

can be left blank and a constant value can be entered in the **Fill** column instead. Alternatively, if one of the property parameters has a matching column of data, the remaining property parameters can be calculated using the values from the matched parameter.

For example, if a data source file contains only horizontal hydraulic conductivity values, the **Kx** value should be matched to this column, while the **Fill** column can be used to set the **Ky** value equal to **Kx** by entering the formula **$KX**. Similarly, the **Kz** value can be defined as one-tenth the **Kx** value using the formula **$KX/10**.



Required Data	Match to column number...	Fill
Comments	1	
X-Coordinate	2	
Y-Coordinate	3	
Kx	5	
Ky	n/a	$KX
Kv	n/a	$KX/10

No.	Name #1	X #2	Y #3	Z #4	Kx #5	Kv #6
2	OW-1	100	100	20	1	2
3	OW-2	750	100	20	2	1
4	OW-3	1500	100	20	2	1
5	OW-4	1900	100	20	1	2

Note: All formula values must use a "**$**" in front of the variables.

The **Source data preview** table shows a preview of the data points which will be interpolated to create the distributed value property zone(s). Each column header is labelled as **Column #N**, where "**N**" is the column number in order from left to right. If the **Use column names from line:** option is used, the default column header will be replaced with the text from the specified line number, but the column number remains.

Once all of the required fields have been matched, press the **[Next]** button to advance to the next step.

Step 3: Data Validation

The third step of the Property Data Import Wizard involves validation of the data being imported. This step will ensure that the data set contains valid data for each of the parameters, and it will ensure the data points are within the model domain. The data validation rules for each model parameter are as follows:

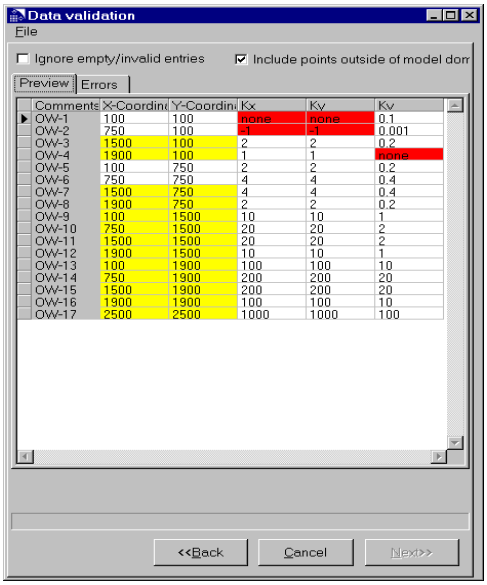
Conductivity

- X-Coordinate [Real Number] / [Required]
- Y-Coordinate [Real Number] / [Required]
- Kx [Positive Real Number]
- Kx/Ky [Positive Real Number]
- Kx/Kz [Positive Real Number]

Storage

- X-Coordinate [Real Number] / [Required]
- Y-Coordinate [Real Number] / [Required]
- Ss [Positive Real Number]
- Sy [Positive Real Number, less than TotPor]
- EffPor [Positive Real Number, less than TotPor]
- TotPor [Positive Real Number, less than one]

A screen capture of **Data Validation** window is shown in the following figure, and the functionality and options for this step are described below.



The **Preview** tab provides a listing of the data points and parameter values which will be interpolated to create the distributed value property zone(s). Invalid data or empty data values will be highlighted in red, while data points located outside the model domain will be highlighted in yellow.

If empty or invalid entries are detected in any of the data points, the offending cells will be highlighted in red and the **[Next]** button will be disabled. The **[Next]** button can be enabled by selecting the **Ignore empty/invalid entries** option.

Data points outside the model domain can be either included in the interpolation, or they can be ignored. To include these data points, select the **Include points outside of model domain** option.

The **Errors** tab provides a description of the errors and warnings for each data point.

Once the data has been validated, press the **[Next]** button to advance tithe next step.

Step 4: Interpolation Options

The **Interpolation Options** step involves:

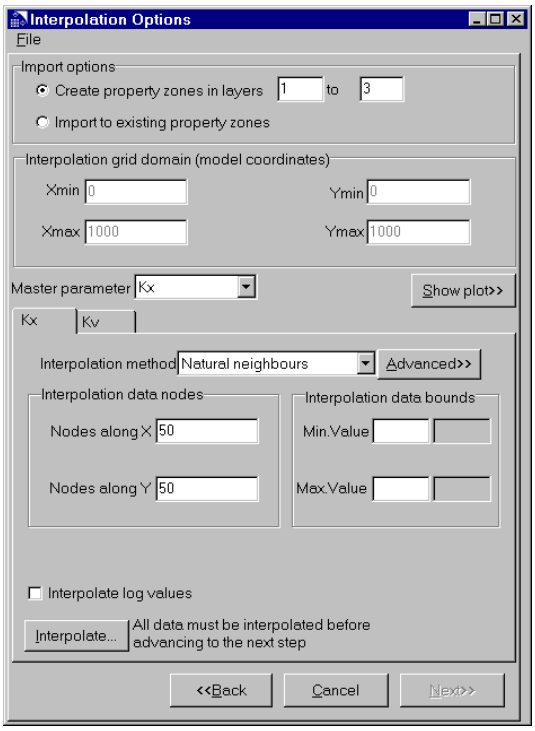
- choosing the destination of the interpolated property data within the model domain,
- selecting the interpolation method and settings
- interpolating the data and creating a distribution array for each parameter

A screen capture of the **Interpolation Options** screen is shown in the following figure, and a description of the features and functionality is provided below.

The **Import Options** frame provides two options for importing the interpolated data into Visual MODFLOW:

- **Create property zones** will create a new property zone(s) in the specified layer(s) and will replace the existing property zone(s) in this layer(s).[1]
- **Import to existing property zones** will populate the grid cells from an existing property zone(s) with the parameter values from the distribution arrays. In this case, no new property zones will be created in the model.

The **Interpolation grid domain** frame shows the spatial dimensions of grid being generated for the interpolated data (in model coordinates). At the present time, these dimensions cannot be modified and the spatial dimensions of the interpolation grid will always correspond to the model dimensions.



The **Master parameter** option is only applicable if:

- the property data being imported has more than one associated parameter (e.g. Conductivity has Kx, Ky and Kz parameters associated with each property zone)
- the **Create property zones in layers** option is selected
- multiple property zones will be created within the selected layer(s).

For presentation purposes, each model property zone is represented by a different color. This makes it easier to identify different soil types within the model domain. However, some of the model property zones require data for multiple parameters (e.g. a Conductivity zone requires values for Kx, Ky and Kz). As a result, when data is being imported for a model property containing more than one parameter, it is necessary to select the **Master** parameter used for defining the range of values associated with each property zone created for the different distribution arrays.

For example, if Conductivity data is imported using separate data points for both Kx and Kz, the distribution of Kx values in the Kx distribution array will be different than the distribution of Kz values in the Kz distribution array. However, both parameters belong to the same set of property zones. The **Master** parameter defines which distribution array will be used to define the range of values assigned to each property zones. If only one property zone is created for the entire distribution array, then the Master parameter is not relevant.

This concept will become clearer in the next step of the Interpolation Wizard.

---

1. If multiple layers are specified, the same distribution array will be applied to each layer.

Interpolation Options

A distribution array must be created for each parameter described by the model property by interpolating the parameter data from the source data file. A separate interpolation options tab is created for each parameter being imported because separate distribution arrays are generated for each parameter.

> **Note:** If a **Fill** value is used to define a parameter, no interpolation is required for this parameter because the distribution array consists of a constant value or a formula applied to a related distribution array.

The **Interpolation Method** field provides a selection of three popular methods of interpolating the data:

- **Inverse distance**
- **Kriging**
- **Natural Neighbor**

The default setting is **Natural Neighbor** because this is a very robust and versatile interpolation method. However, **Kriging** is also a very popular interpolation method for geoscience applications.

The **[Advanced]** button opens the **Interpolation options** window with access to more advanced settings for the selected interpolation method. A general description of each method and a detailed description of the advanced settings for each of these methods is provided in Appendix B.

Interpolation data nodes

The **Interpolation data nodes** frame describes the number of nodes in the **X** and **Y** direction for the interpolation grid used to create the distribution array. It is important to note that the interpolation grid density is NOT dependent on the model grid spacing, but rather on the density of the data points. If the data points are very closely spaced in a particular region of the model, the grid spacing should be small, and the number of grid nodes should be large. However, if the data points are well distributed and relatively well-spaced, then the grid spacing can be large, and the number of grid nodes should be small.

Obviously, large interpolation grids create large data files and take longer to process. Therefore, the number of interpolation data nodes should be as low as possible.

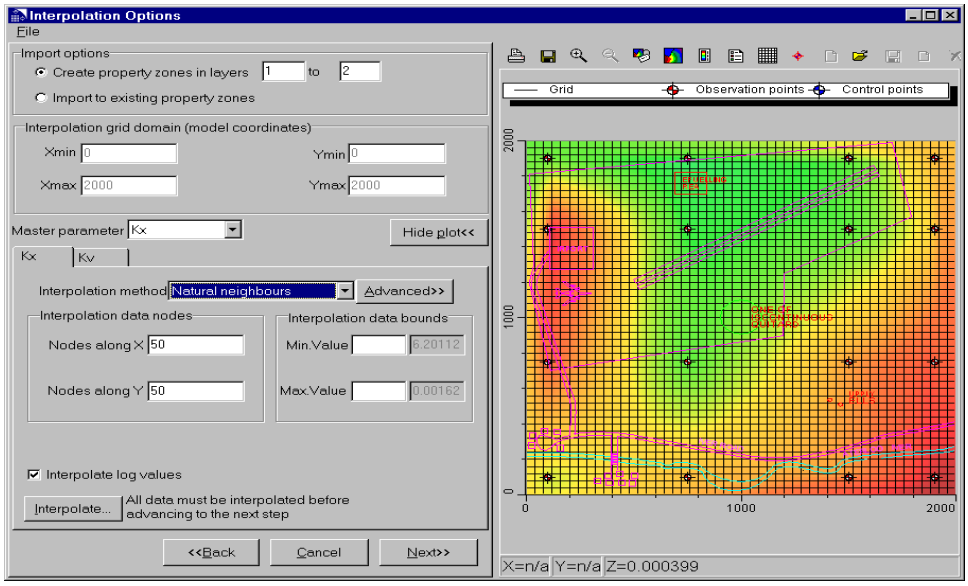
Interpolation data bounds

The **Interpolation data bounds** frame describes the minimum and maximum values for the interpolated data and allows for user-defined minimum and maximum values. The reason these fields are required is to avoid importing invalid data that is sometimes created when interpolating field data points. For example, a data set for hydraulic conductivities may contain all positive values, but a spatially decreasing trend may cause the interpolation scheme to “predict” negative conductivity values in a certain region of the model domain. The **Minimum value** and **Maximum value** fields allow the user to control the absolute minimum value predicted by the interpolation scheme. If a

value is predicted below the **Minimum value**, it is assigned equal to the **Minimum value**.

The **Interpolate log values** option will interpolate the log values of the data points and then invert the log value distribution. This option is commonly used for interpolating data with a high degree of variance such as hydraulic conductivities and initial concentrations.

The **[Interpolate]** button is used to start the interpolation process and create the distribution array for the selected parameter. A preview of the distribution array can be seen by clicking the **[Show Plot >>]** button to open a new panel showing color map of the distribution array as shown in the following figure.



Control Points

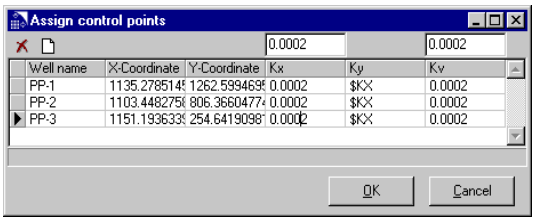
In many situations, the interpolated distribution of data does not properly represent the actual situation in the field. In some situations, it may be necessary to 'guide' the interpolation of the data by adding Control Points at strategic locations.

Adding Control Points

Interpolation control points can only be added in the Plot panel by clicking the **Add control point(s)** icon in the toolbar at the top of the window. Then left-click the mouse pointer on the desired control point location(s) within the interpolation grid domain. A blue and red station symbol will appear at each control point location.

Once the control points have been added in the desired locations, right-click on the plot or click the **Assign control point(s)** data icon to enter the parameter values for each control point. The **Assign control points** window will appear as shown in the following figure.

The **Assign control points** dialog contains a table listing the attributes for each control point.



The **Station ID** is automatically assigned to each control point in the order they are created

The **X-Coordinate** and **Y-Coordinate** are automatically assigned to each control point based on the location where they are added to the plot

The required parameter values will depend on the property data being imported and the parameter data being interpolated

Each control point requires a complete set of valid parameter values.

Additional control points can be added to the table by clicking the **[Add control point(s)]** icon in the toolbar of the **Assign control points** window and entering the required information in the blank line.

Alternatively, control points can be deleted from the table by selecting the row and clicking the **Delete control points** icon in the toolbar of the **Assign control points** window.

Editing Control Points

Once the control point(s) data has been entered, the control points data can be modified by clicking the **[Edit control point(s)]** icon on the toolbar. The **Edit control points** window has the same functionality as the **Assign control points** window.

Saving Control Points Data

The control point(s) data can be saved to a text file by clicking the **[Save control points]** icon on the top toolbar. This data can be saved for easily loading this data later on or reporting the control point data in a report.

Loading Control Point Data

If a previous interpolation needs to be re-done or slightly modified, the control point data from a previous session may be re-loaded by clicking the **[Load control points]** icon on the top toolbar.

Deleting Control Points

Control points can be deleted by clicking the **[Delete control point(s)]** icon in the top toolbar and mouse pointer on the control points to delete.

Once each parameter data set has been interpolated and a suitable distribution array has been created for each, click the **[Next]** button to advance to the next step.

If the **Import option** in Step 4 is set to **Create new property zones** then proceed to section Step 5a: Create Property Zones on page 82.

If the **Import option** in Step 4 is set to **Import to existing property zones** then proceed to section Step 5b: Select Property Zones on page 85.

Step 5a: Create Property Zones

A screen capture of the **Create Property Zones** window is shown in the following figure and the functionality and features of this step are described below.

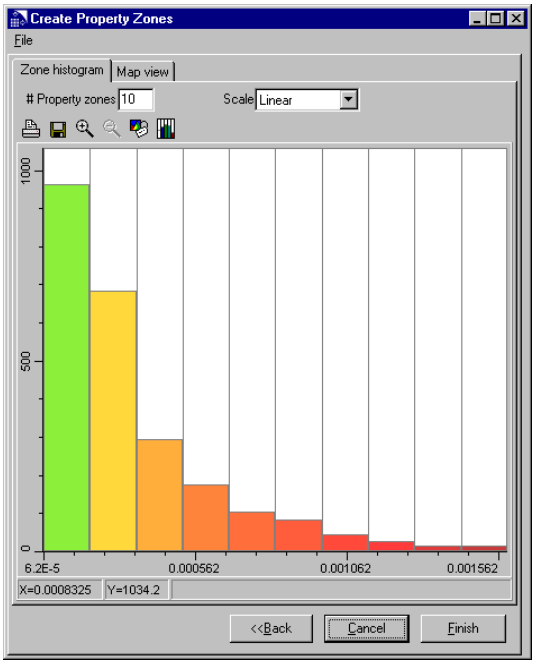
The interpolated data for each parameter is stored in a parameter distribution array having the same X-Y dimensions as the model domain (as described in section Distributed Value Property Zones on page 70). When new property zones are created for the imported data, the zone parameter values for each new property zone are each assigned a unit value (i.e. 1.0). The property values assigned to each grid cell within that property zone are calculated by multiplying the zone parameter value (1.0) with the corresponding value from the parameter distribution array.

The **Create Property Zones** step is used to define the number of property zones that will be created for the selected layers, and to customize the range of values represented by each property zone.

> **Note:** The number of property zones created will NOT affect the property values assigned to each grid cell, but it will make it easier to identify cells within a certain range of values, and uniformly modify the parameter values for selected zones.

The **Zone histogram** tab displays a histogram of the property zones as shown in the following figure. The X-axis displays the range of values for the **Master parameter**, and the Y-axis displays the number of model grid cells associated with each zone. Since each property zone may contain data for several different parameters, the **Master parameter** (defined in section Step 4: Interpolation Options on page 77) is used to determine the range of values represented by each zone. The default setting creates 10 different property zones, each with the same increment value along the x-axis.

The **# Property zones** field indicates the number of property zones to create. This field can be customized to create just one property zone or hundreds of property zones.



In many situations it will be sufficient to create only a single property zone representing the entire range of property values for the entire layer or set of layers. This will make it easy to uniformly increase or decrease the property values for the entire layer during the calibration process. However, if there is a specific region of the model where higher or lower ranges of property values make it more sensitive, then it may be useful to create several different property zones to effectively 'isolate' the more sensitive regions.

Setting the Scale for the Zone Values Axis

The **Scale** option controls the scale of the zone value axis (the X-axis) on the Zone histogram. The default setting is **Linear**. However, if the **Master parameter** ranges over several orders of magnitude, it may be easier or more appropriate to delineate the range of values associated with each property zones using a Log scale.

Customizing the Range of Values for Each Property Zone

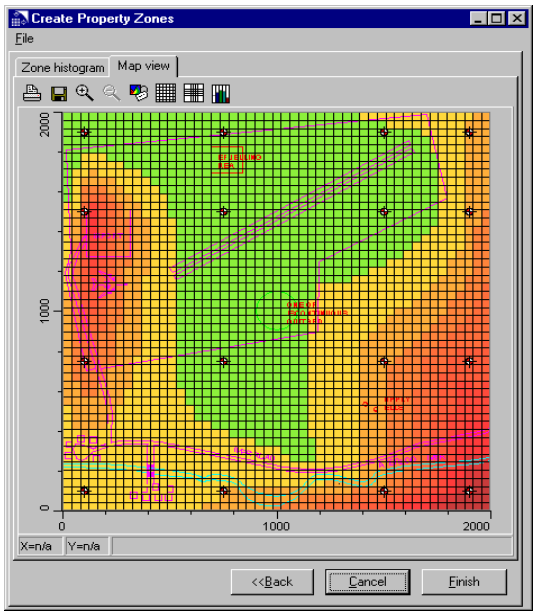
When the **# Property zones** value is entered, the default setting is to create uniform increments for each property zone. However, this does not always yield the desired distribution of property zones. The range of values for each property zone can be customized by clicking-and-dragging the vertical line bounding each bar on the histogram to a new position along the x-axis.

Customizing the Zone Colors

The default display setting for the histogram shows a rainbow color scale for the bars representing the property zones. Unfortunately, this rainbow color scale does not match the property zone colors that will be used in the Visual MODFLOW model grid. The current version of Visual MODFLOW does not allow customized property zone colors, but the actual property zone colors for each zone can be displayed by clicking the **[Zone colors]** icon in the toolbar above the histogram.

Mapping Zones to the Model Grid

The **Map view** tab displays a preview of the property zone distribution in the model domain as shown in the following figure. The default display settings show the distribution array grid using a rainbow color gradient for the zones.



The property zone colors, as they will appear in Visual MODFLOW, can be displayed by clicking the Visual MODFLOW colors icon in the toolbar above the map.

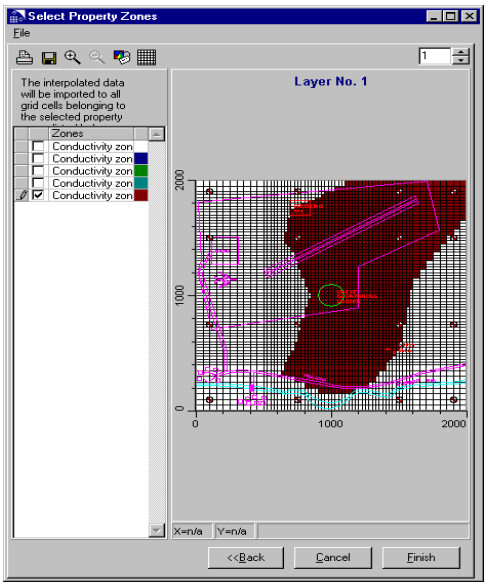
The property zone distribution on the actual model grid can be displayed by clicking the **[Model grid]** icon in the toolbar above the map.

Once the desired property distribution has been achieved, press the **[Finish]** button to import the new property zone data into the Visual MODFLOW model.

> **Hint:** If several property zones were created for this data set it is a good idea to print the Zone histogram before pressing the **[Finish]** button. The Zone histogram provides a reference for the range of values represented by each zone.

Upon returning to the Visual MODFLOW screen a message will appear asking "**Remove unused property zones?**". If the new property zone(s) created for the specified layers of the model is replacing an existing zone(s), the previous zone will be removed from the list of zones if it is not longer being used anywhere else in the model.

Step 5b: Select Property Zones



The **Import to existing property zones** options effectively "links" the selected property zones to the associated parameter distribution arrays. In doing so, the original zone parameter value is replaced by a unit parameter value (1.0). The property values assigned to each grid cell within that property zone are calculated by multiplying the zone parameter value (1.0) with the corresponding value from the parameter distribution array.

The left-hand side of the window lists all of the available property zones with an empty checkbox beside each one. If a property zone is selected, it will appear on the **Map preview** panel. If the selected zone does not appear on the map, use the **View Layer** control to view the model layer where this property zone is located.

When the desired property zones have been selected, press the **[Finish]** button to import the interpolated property data into the Visual MODFLOW model.

Assigning Property Zones

As discussed on page 70, the Constant Value Property Zone approach is the fastest and easiest way to define the model properties. Although Visual MODFLOW supports an unlimited number of property zones, the usual practice is to develop a simplified conceptual model with only a few different property zones, and then add more property zones as necessary to calibrate the model.

Property zones can be assigned to the model grid cells using one of the **[Assign >]** options from the left-hand toolbar.

- **[Assign >] Single** is used to select individual grid cells where the property zone will be assigned. Hold the mouse button down to select multiple grid cells, and press the right mouse button to unselect grid cells.
- **[Assign >] Polygon** is used to digitize a polygon around the group of grid cell where the property zone will be assigned. Left-click at the start point of the polygon to begin digitizing the shape of the polygon and right-click near the start point to close the polygon.
- **[Assign >] Window** is used to stretch a rectangular window around the group of grid cells where the property zone will be assigned. Left-click at one corner of the window and left-click again at the opposite corner to define the window

dimensions.

Once the grid cells been selected using one of the [Assign >] options described above, an **Assign Property** dialog window will appear as shown in the following figure.

The **Assign Property** window is used to assign a property zone to the grid cells inside the polygon. This window shows the property zone number and color, and the parameter values associated with this property zone.

A different property zone can be selected by typing a zone number (integer value) into the **Property #** field, or by clicking the up or down arrow buttons ( ) to scroll through the list of available property zones.

If none of the available property zones have the appropriate set of parameter values, a new property zone can be created by clicking the **[New]** button and entering the new parameter values.

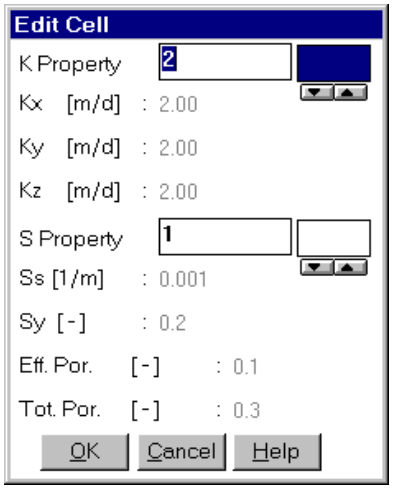
Editing Property Zones

Visual MODFLOW provides two different options for editing the property zones assigned to the model grid:

- **[Edit >] Single**
- **[Edit >] Property**

Edit Single

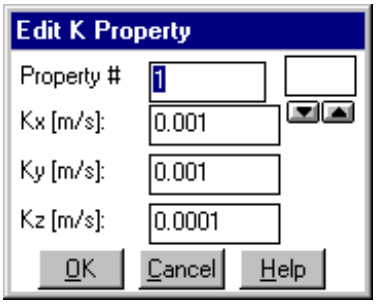
The **[Edit >] Single** option is used to change the property zone assigned to a few selected grid cells. When the **[Edit >] Single** option is chosen, use the mouse pointer to click on the target grid cell to change and an **Edit Cell** dialog window will appear as shown in the figure on the right.



The **Edit Cell** dialog will show the relevant property zone data associated with the selected grid cell. Use the up or down arrow buttons ( ) to change the property zone data assigned to this grid cell.

Edit Property

The **[Edit >] Property** option is used to actually change the parameter values for a selected property zone. When **[Edit >] Property** is chosen, an **Edit Property** dialog window will appear as shown in the figure below.



The **Edit Property** dialog shows the property zone number and color, and the parameter values associated with this property zone. If the parameter values are changed, these changes will be applied to all model grid cells associated with this property zone.

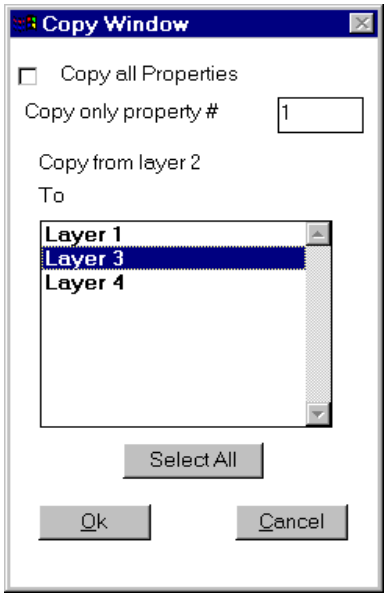
Although the **[Edit >] Property** option is useful for modifying selected property zones, the **[Database]** option provides a more convenient method for viewing and modifying the parameter values for all of the property zones in the model. The features and functionality of the Property Database is described below.

Copying Property Zones

In many instances, a multi-layer model will be constructed where a single aquifer unit occupies multiple model layers. In this case, the property zone distribution for one layer can be copied to the other layers to avoid the repetitive task of re-assigning the property zone distribution for each layer. Visual MODFLOW provides an option for copying either all property zones or a specified property zone from the current layer, row or column, to one or more layers, columns or rows.

The sub-menu option for the **[Copy >]** button will depend on the current view of the model. For example, if the active model view is a layer then the sub-menu will be **[Copy >] Layer**, if the active model view is a row then the sub-menu will be **[Copy >] Row**.

To copy the entire property zone distribution in the current layer to another layer, or set of layers, select [Copy] > [Layer] and a **Copy Window** will appear listing the other layers of the model and the options for defining which property zones to copy.



The **Copy All Properties** option will copy the entire property zone distribution from the current layer to the destination layer(s).

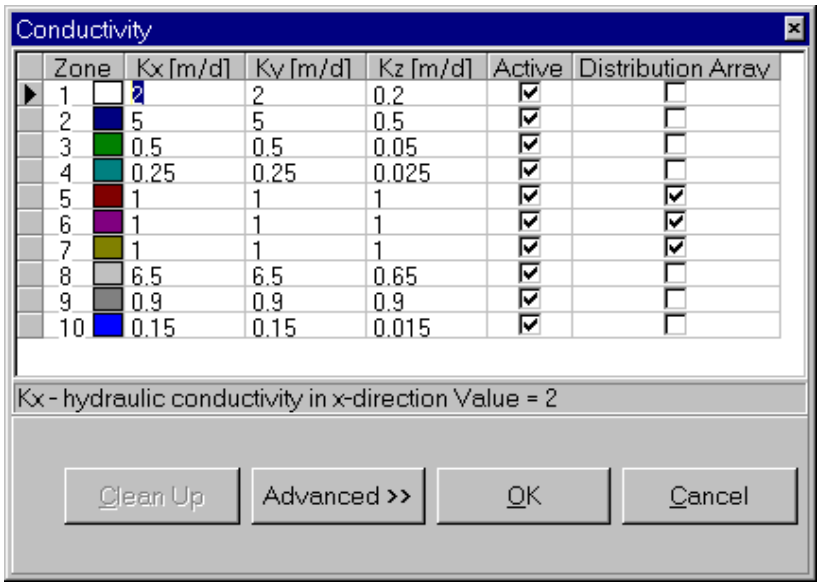
The **Copy only property #** __ option will copy only the specified property zone from the current layer to the destination layer(s).

The destination layer(s) can be chosen by clicking on the target layers in the list. Multiple layers can be chosen by holding down the **<Ctrl>** key while clicking.

The **[Select All]** button will choose all layers in the list.

Editing the Property Database

The **[Database]** button loads the **Property Database** window as shown in the following figure. The **Property Database** window is used for viewing and editing the parameter values and settings for all property zones in the model. The functionality and settings for the property zones are described below.



Each row of the **Property Database** table contains information about each of the model property zones including:

- Zone number and associated color
- Zone parameter values
- Active setting
- Distribution Array link setting

The status bar below the table panel displays information about each zone parameter value by simply clicking the cursor on the zone parameter of interest.

The **Zone** numbers and colors are read-only data and cannot be modified.

The zone parameter values can be modified by simply entering a new value in the desired field.

The **Active** setting indicates whether the zone active or inactive. An inactive zone is not assigned to any grid cells in the model and may be removed without affecting the model results. Inactive zones can be removed using the **[Cleanup]** button.

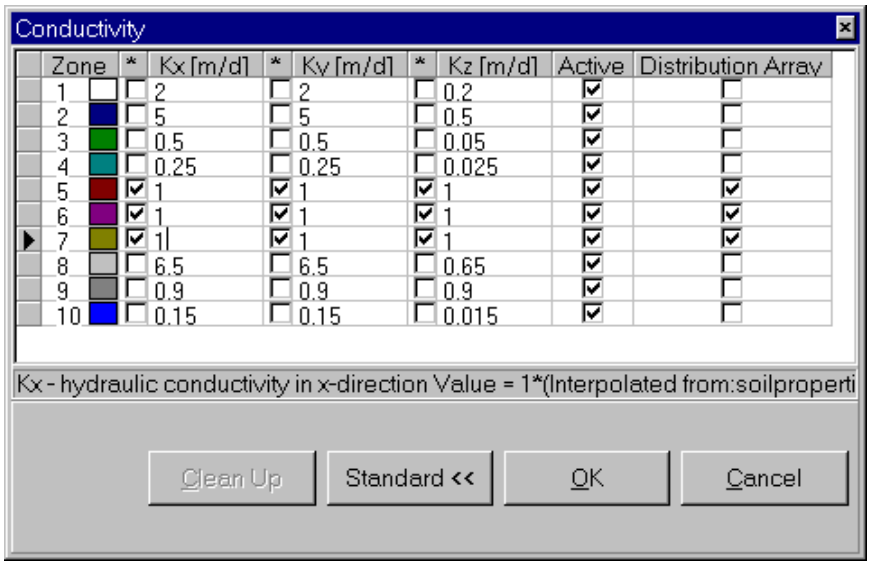
The **Distribution Array** setting can be turned ON or OFF.

If the **Distribution Array** setting is ON, the zone parameter values from the database will be multiplied with the values from the associated distribution array to calculate the property values assigned to each grid cell. A more detailed explanation of the Distributed Property Value approach is provided on page 70.

If the **Distribution Array** setting is OFF, the zone parameter values from the Property Database will be assigned to each grid cell associated with this property zone.

The **[Cleanup]** button is used to remove unused property zones from the database and to re-index the property zones in ascending order. This cleanup will likely cause some changes in the appearance of the property zone distributions because the zone colors are linked to the zone numbers. However, it will not affect the model results because the property values assigned to each grid cell does not change.

The **[Advanced]** button switches to the advanced view of the **Property Database** window. The **Advanced** view provides the additional option of changing the **Distribution Array** settings for each individual zone parameter as shown in the following figure.


Conductivity
Zone * Kx [m/d] * Ky [m/d] * Kz [m/d] Active Distribution Array
1 2 2 0.2
2 5 5 0.5
3 0.5 0.5 0.05
4 0.25 0.25 0.025
5 1 1 1
6 1 1 1
7 1 1 1
8 6.5 6.5 0.65
9 0.9 0.9 0.9
10 0.15 0.15 0.015
Kx - hydraulic conductivity in x-direction Value = 1*(Interpolated from:soilproperti
Clean Up
Standard <<
OK
Cancel

Contouring Property Data

The ability to display contour maps and color maps of the model property values assigned to each grid cell is particularly useful now that distributed model properties can be imported and interpolated to the model grid.

The **[Contouring >]** option contains a sub-menu listing the available parameters to contour, and an **Options** selection is available to customize the appearance of the contour map and/or color map. The features and functionality of the contour options window is described in the section Contour Map Display Options on page 230.

To remove the contour map and/or color map for a property parameter, select **[Contouring >]** and then select the parameter name to remove. Notice when the contour display option is set to ON a ✓ appears beside the parameter name, and when it is set to OFF the ✓ disappears.

3.4.2 Conductivity

The **Conductivity** screen is used to view, assign, edit, copy and contour the Conductivity (hydraulic conductivity) parameter values of the model including:

- **Kx** - hydraulic conductivity in the direction of the model X-axis
- **Ky** - hydraulic conductivity in the direction of the model Y-axis
- **Kz** - hydraulic conductivity in the direction of the model Z-axis

These **Conductivity** parameters may be defined on a cell-by-cell basis using constant property values and/or distributed property values (see descriptions on page 70). When

importing or assigning the Conductivity property zones, Visual MODFLOW will require valid data for each of the above parameters.

When entering the **Conductivity** screen for the first time, a **Default Properties** dialog will appear prompting for default conductivity and storage parameters. These default parameter values will be assigned to **Property Zone #1** and will be applied to all grid cells in the entire model domain.

The graphical tools for importing, assigning, editing, copying and contouring Conductivity property zones and parameter values are located along the left-hand menu bar and are described in detail in the section Tools for Assigning and Editing Properties on page 72.

Anisotropy

The reason Visual MODFLOW prompts for both **Kx** and **Ky** is because there are two options for defining the horizontal anisotropy of the Conductivity property zones:

- Anisotropy by layer
- Anisotropy as specified

Note: The anisotropy option is set in the **Run** section under the **MODFLOW > Anisotropy** menu item (see description on page 179).

If the **Anisotropy by layer** option is used, the **Kx** value will determine the conductivity in the X-direction, and the specified anisotropy ratio (**Ky/Kx**) for each layer will be used to calculate the **Ky** value for each grid cell.

If the **Anisotropy as specified** option is used, the model will use the **Kx** and **Ky** values defined for each property zone.

Calculating Transmissivity and VCONT

Visual MODFLOW does NOT prompt for Transmissivity or VCONT values because the geometry of each model layer is required to be explicitly defined. As a result the Transmissivity and VCONT values are automatically calculated by Visual MODFLOW during the translation from Visual MODFLOW file formats to MODFLOW input data files (as discussed in Chapter 4).

3.4.3 Storage

The **Storage** screen is used to view, assign, edit, copy and contour the Storage parameter values of the model including:

- **Ss** - specific storage
- **Sy** - specific yield
- **EffPor** - effective porosity
- **TotPor** - total porosity

Specific Storage (Ss) is defined as the volume of water that a unit volume of aquifer releases from storage under a unit decline in hydraulic head. Using Specific Storage, Visual MODFLOW determines the primary storage coefficient (sf1) for MODFLOW. The primary storage coefficient is calculated by Visual MODFLOW to be equal to the specific storage multiplied by the layer thickness.

Specific Yield (Sy) is known as the storage term for an unconfined aquifer. It is defined as the volume of water that an unconfined aquifer releases from storage per unit surface area per unit decline in the water table. For sand and gravel aquifers, specific yield is generally equal to the porosity.

Effective Porosity (EffPor) is the pore space through which flow actually occurs and used by MODPATH to determine average linear groundwater velocities for use in time-dependent capture zones and time markers along pathlines. This term is not used for MODFLOW simulations.

Total Porosity (TotPor) is the total pore space of the porous media and is used in MT3D to determine the chemical reaction coefficients and for calculating the average linear groundwater flow velocity in the particle tracking solution schemes. A different porosity might be used for MT3D than for MODPATH because MT3D accounts for additional transport and reactive processes, such as dispersion. The total porosity term is not used for MODFLOW simulations.

These **Storage** parameters may be defined on a cell-by-cell basis using constant property values and/or distributed property values (see descriptions on page 70). When importing or assigning the **Storage** property zones, Visual MODFLOW will require valid data for each of the above parameters.

When entering the **Storage** screen for the first time, a **Default Properties** dialog will appear prompting for default **Conductivity** and **Storage** parameters. These default parameter values will assigned to **Property Zone #1** and will be applied to all grid cells in the entire model domain.

The graphical tools for importing, assigning, editing, copying and contouring Storage zones and parameter values are located along the left-hand menu bar and are described in detail in the section Tools for Assigning and Editing Properties on page 72.

Copying the Conductivity Zone Distribution

In most situations, the porous media zones having different **Conductivity** parameters will also have different **Storage** parameter values. As a result, Visual MODFLOW provides the option of copying the **Conductivity** property zone distribution to the **Storage** input screen. This avoids the tedious task of trying to manually duplicate the **Conductivity** property zone arrangement with the **Storage** property zones.

To copy the **Conductivity** zones distribution, select **[Copy >] Distrib** from the side menu bar and the **Storage** property zones will automatically be created for every hydraulic conductivity zone (the values of the storage parameters for all new storage zones will be automatically set to the default **Storage** parameter values).

Next, select the **[Database]** button from the side menu bar and modify the storage values for each zone as needed.

3.4.4 Initial Heads

In order to start solving the flow simulation MODFLOW requires an initial “guess” for the head values in the model. A good initial guess for the starting heads of the simulation can reduce the required run time significantly. The Initial Head values are also used to calculate the drawdown values, as measured by the difference between the starting head and the calculated head.

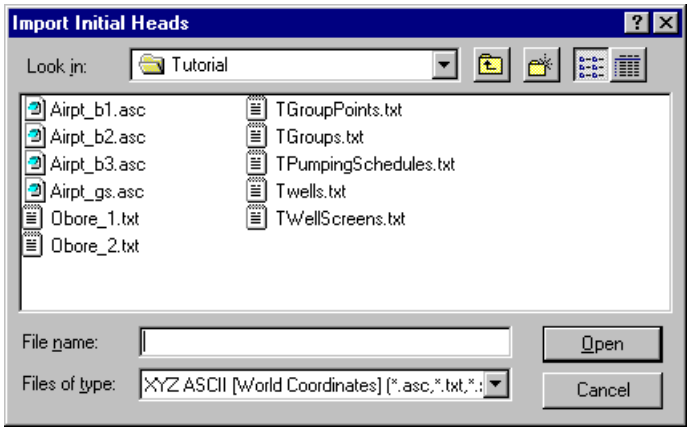
The **Initial Heads** screen is used to view, assign, edit, copy and contour the initial head values. The graphical tools for assigning, editing, copying and contouring Initial Head zones and values are located along the left-hand menu bar and are described in detail in the section Tools for Assigning and Editing Properties on page 72.

Importing Initial Heads

Currently, the **Initial Head** values in the Input section of Visual MODFLOW can only be defined on a cell-by-cell basis using the Constant Property Value approach. Support for distributed property values will be added for Initial Heads in future releases.

However, the **Initial Heads** screen also has an **[Import]** button that uses a constant property value approach to dealing with imported data.

To import initial heads data, select **[Import]** from the side menu bar. The following **Import Initial Heads** window will appear.



Select the type of file to import by pressing on the down arrow for the **Files of type** picklist. Visual MODFLOW can import initial heads data from the following file formats:

- **XYZ ASCII (World or Model co-ordinate systems)** - must be three columns of tab, comma or space delimited data (X, Y, Head) without column headers
- **Surfer™ Grid (World or Model co-ordinate system)** - binary .GRD file only
- **Previous MODFLOW Run** - .HDS file must be from a model with the same grid configuration as the current model

Depending on the type of file chosen, some or all of the following information will be required:

- **Nearest Neighbours** is the number of nearest data points used in the inverse difference weighted linear interpolation.
- **Import Tolerance** is the property value defining the difference in property zones (the default value is ± 0.01 property units). If the tolerance is set low then there will be many values and the initial heads will be representative of the conditions, but the database will be huge. If the tolerance is set high then there will not be many zones and the initial heads will not be as representative of the exact conditions. To avoid this problem refer to the Initial Heads description in the **Run** section on page 162. In the **Run** section, exact values are used since there is no placement of the data into a database.
- **Select Output Time** is used to select the Output time of the previous MODFLOW run. If the model was run in transient mode, the desired Output time may be selected from the list of times and timesteps. If the model was run in steady-state mode, only one Output time will be listed.

3.4.5 Bulk Density

The soil Bulk Density is used to calculate the Retardation Coefficient (R) for each chemical species according to the following formula:

$$R_i = 1 + \frac{p_b}{n} \times K_{d(i)}$$

Where;

R_i = Retardation Coefficient of Species i (unitless)

p_b = Soil Bulk Density (in units of M/L^3)

n = Effective Soil Porosity (in units of L^3/L^3)

$K_{d(i)}$ = Distribution Coefficient of Species i (in units of L^3/M)

The Retardation Coefficient is used to calculate the 'retarded' flow velocity ($v_{R(i)}$) of each chemical species according to the following formula:

$$v_{R(i)} = \frac{v}{R_i}$$

Where;

$v_{R(i)}$ = Retarded Flow Velocity of Species i (in units of L/T)

v = Groundwater Flow Velocity (in units of L/T)

R_i = Retardation Coefficient of Species i (unitless)

The retarded flow velocity is used to calculate the advective transport of each species.

Unless otherwise specified during the setup of the Transport Variant, the default soil Bulk Density value for any new model created in Visual MODFLOW is 1700 kg/m^3.

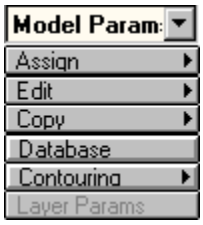
The options for customizing the soil Bulk Density values will depend on which Transport Engine is selected for the current transport variant. The following is a summary of the graphical tools available for assigning Bulk Density for each of the available Transport Engines (assuming a sorption method is selected).

- For MT3D96, MT3DMS, MT3D99and RT3Dv2.5, the soil Bulk Density is assigned on a cell-by-cell basis and all graphical tools are available.
- For MT3Dv1.5 and RT3Dv1.0, the soil Bulk Density is Layer Parameter and cannot be specified on a cell-by-cell basis.

The graphical tools for assigning, editing, and copying Bulk Density values are located along the left-hand menu bar and are described in detail in the section Tools for Assigning and Editing Properties on page 72.

If no sorption method is used in the current Transport Variant, then no Bulk Density values are required for the simulation and all of the options in the left-hand toolbar will be disabled.

3.4.6 Model Params. (Transport)



The **Model Params. (Transport)** screen is only available for models where RT3D is the Transport Variant *and* the Reactions model is spatially variable (these setting are specified during the setup of the Transport Engine as described in the section Mass Transport Numeric Engine on page 25). The **Model Params. (Transport)** screen is used to define the soil Bulk Density and the reaction parameters required for the selected Reaction model (the reaction parameters required for each reaction model are described in Appendix C).

The graphical tools for assigning, editing, copying and contouring the Reaction model parameters are located along the left-hand menu bar and are described in detail in the section Tools for Assigning and Editing Properties on page 72.

3.4.7 Species Parameters

The Species Parameters screen is used to specify the sorption and reaction parameters used by the selected Transport Engine. Each of the Transport Engines can handle a different set of sorption methods and reactions, so the options for customizing the sorption and reaction parameters will depend on which Transport Engine is selected for the current Transport Variant (see Appendix C for a summary of the available sorption options for each Transport Engine).

The following is a summary of the graphical tools available for assigning sorption and reaction parameters for each of the available Transport Engines (assuming a sorption method and a reaction model are selected).

- For MT3D96, MT3DMS, and MT3D99 the sorption and reaction parameters are assigned on a cell-by-cell basis and all graphical tools are available.
- For MT3Dv1.5 the sorption and reaction parameters are assigned as Layer Parameters and cannot be specified on a cell-by-cell basis.
- For RT3Dv1.0 only the sorption parameters are assigned as Layer Parameters and cannot be specified on a cell-by-cell basis
- For RT3Dv2.5 only the sorption parameters are assigned on a cell-by-cell basis and all the graphical tools are available.

The graphical tools for assigning, editing, and copying Bulk Density values are located along the left-hand menu bar and are described in detail in the section Tools for Assigning and Editing Properties on page 72.

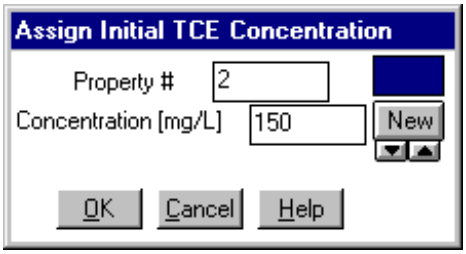
If no sorption or reactions are selected in the current Transport Variant, then no sorption or reaction parameters are required for the simulation and all of the options in the left-hand toolbar will be disabled.

Contouring Option

The contouring overlays specific to the chemical reactions property are the First Coefficient Contour, the Second Coefficient Contour, the Bulk Density Contour, the Dissolved Decay Rate Contour, and the Sorbed Decay Rate Contour. To view an overlay, select **[Contouring]** and then the desired overlay from the sub-menu. Note, only one overlay can be viewed at a time. If the current contour is not toggled off and another one is selected, the newly selected contour will become the toggled on contour. To remove the contours, select **[Contouring]** and the current overlay.

3.4.8 Initial Concentration

In many cases the historical conditions of the site are unknown and the contaminant source has been removed or remediated. However, the groundwater contamination is still present and the mass transport simulation must be run forward in time, starting from the existing conditions, to predict the potential downstream impacts. The **Initial Concentration** input screen is used to define the existing conditions (concentrations) of each chemical species being simulated.



The **Initial Concentration** input screen is used to view, assign, edit, copy and contour the initial concentration values (existing conditions) for each chemical species being simulated. The graphical tools for assigning, editing, copying and contouring Initial Concentration zones and values are located along the left-hand toolbar and are described in detail in the section Tools for Assigning and Editing Properties on page 72.

Importing Initial Concentrations

The **Initial Concentrations** input screen does not currently have an option for importing and interpolating Initial Concentration values from an external file. However, Initial Concentration values can be imported in the **Run** section of Visual MODFLOW (see section Importing Initial Concentrations on page 196).

Assigning Inactive Transport Zones

In many cases, the area of interest for the mass transport simulation will occupy only a small subregion of the model domain. As a result, it is not necessary to include the entire model domain and all of the associated grid cells in the mass transport model calculations. Visual MODFLOW provides an option for graphically assigning regions of the model outside the zone of interest as Inactive For Transport. MT3D does not simulate contaminant transport through cells defined to be Inactive For Transport.

The Inactive For Transport regions of the model are defined by selecting one of the **[Inactive Trans.]** options from the left-hand toolbar.

Mark Poly. Active Digitize a polygon around a group of cells which will be designated as active. Left-click at the start point of the polygon to start digitizing the shape of the polygon and right-click near the start point to close the polygon.

Mark Inactive Digitize a polygon around a group of cells which will be designated as inactive (indicated by a solid black color). Left-click at the start point of the polygon to start digitizing the shape of the polygon and right-click near the start point to close the polygon.

Mark Single Designate grid cells as either active or inactive by clicking on individual grid cells, or by clicking-and-dragging across multiple grid cells. Click the left mouse button to designate cells as inactive, and click the right mouse button to designate cells as active.

Copy Single Copy the active/inactive setting for individually selected grid cells to other layers/row/columns of the model.

Copy Polygon Copy the active/inactive setting for a group of grid cells defined by a polygon to other layers/rows/columns of the model.

If the dissolved mass (solute) reaches a grid cell defined as Inactive For Transport, the groundwater will flow through it but the solute mass will “build-up” on the upstream side of the Inactive For Transport boundary producing some unreasonable results. To avoid this scenario, special care should be taken to avoid placing the Inactive For Transport boundary too close to the region of interest.

3.4.9 Dispersion

Dispersion is a mechanical process that tends to ‘disperse’, or spread, the contaminant mass in the X, Y and Z directions along the advective path of the plume and acts to reduce the mass concentration. Dispersion is caused by the tortuosity of the flowpaths of the groundwater as it travels through the interconnected pores of the soil.

Dispersion is calculated using the equation:

$$D = \alpha_L \times \frac{v_L^2}{|v|} + \alpha_H \times \frac{v_H^2}{|v|} + \alpha_V \times \frac{v_V^2}{|v|} + D^*$$

Where:

D	is the Dispersion
α_L	is the longitudinal dispersivity (units of 1/length)
v_L	is the longitudinal velocity of flow along the plume migration pathway
α_H	is the horizontal dispersivity (units of 1/length)
v_H	is the horizontal velocity of flow along the plume migration pathway
α_V	is the vertical dispersivity (units of 1/length)
v_V	is the vertical velocity of flow along the plume migration pathway
D*	is the diffusion coefficient (no units)

MT3D calculates the Dispersion tensor for the mass transport model using the following parameters:

- Longitudinal Dispersivity for each transport grid cell
- Ratio of Horizontal to Longitudinal Dispersivity for each layer
- Ratio of Vertical to Longitudinal Dispersivity for each layer
- Molecular Diffusion Coefficient for each layer

The **Dispersion** input screen in Visual MODFLOW is used to view, assign, edit, copy and contour the Longitudinal Dispersivity values in the model. The graphical tools for assigning, editing, copying and contouring Longitudinal Dispersivity zones and values are located along the left-hand toolbar and are described in detail in the section Tools for Assigning and Editing Properties on page 72.

The [**Layer Options]** button on the left-hand toolbar is used to define the values for:

- Ratio of Horizontal to Longitudinal Dispersivity for each layer [Default = 0.1]
- Ratio of Vertical to Longitudinal Dispersivity for each layer [Default = 0.01]
- Molecular Diffusion Coefficient for each layer [Default = 0.1]

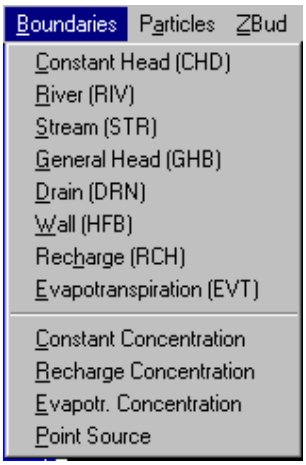
3.5 Boundary Conditions

Every model requires an appropriate set of boundary conditions to represent the system's relationship with the surrounding systems. In the case of a groundwater flow model, boundary conditions will describe the exchange of flow between the model and the external system. In the case of a mass transport model, the boundary conditions will describe the exchange of solute mass between the model and the external system.

In Visual MODFLOW the boundary conditions for the groundwater flow and mass transport model are assigned and edited in the **Boundaries** module of the **Input** section. The **Boundaries** menu items are divided into two sections:

(1) Flow boundary conditions

- **Constant Head (CHD)**
- **Rivers (RIV)**
- **Stream Routing (STR)**
- **General Head (GHB)**
- **Drains (DRN)**
- **Walls (HFB)**
- **Recharge (RCH)**
- **Evapotranspiration (EVT)**



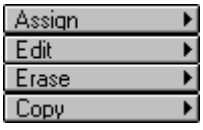
(2) Transport boundary conditions

- **Constant Concentration**
- **Recharge Concentration**
- **Evapotranspiration Concentration**
- **Point Source Concentration**

The groundwater flow boundary conditions are all add-on packages included with both MODFLOW-96 and MODFLOW-2000. Any MODFLOW-2000 boundary condition packages not included in this list may still be run with the model as long as the input files for these packages have the same project name and are located in the same project directory (see section Running Input Files From Unsupported Packages on page 212 for details).

These mass transport boundary conditions are all supported by the various mass transport codes supported by Visual MODFLOW (e.g. MT3Dv.1.5DoD, MT3D-96, MT3DMS, MT3D-99, RT3Dv.1 and RT3Dv.2.5).

3.5.1 Tools for Assigning and Editing Boundary Conditions



In general, each boundary conditions has the same set of graphical tools on the left-hand toolbar for assigning, editing, erasing and copying the model boundary conditions. The following is a description of how to use these options. For specific descriptions of the data requirements and data entry options refer to the section describing each boundary condition type.

[Assign >]

- **[Assign >] Single** is used to select individual grid cells where the boundary condition will be assigned. Hold the mouse button down to select multiple grid cells, or click the right mouse button to unselect grid cells.
- **[Assign >] Line** is used to digitize a line along the path of grid cells where the boundary condition will be assigned. Left-click at the start point of the line and continue to left-click at each node of the line. Right-click at the end point of the line.
- **[Assign >] Polygon** is used to digitize a polygon around the group of grid cells where the boundary condition will be assigned. Left-click at the start point of the polygon to begin digitizing the shape of the polygon and right-click near the start point to close the polygon.
- **[Assign >] Window** is used to stretch a Window (rectangle) around the group of grid cells where the boundary condition will be assigned. Left-click at one corner of the window and left-click again at the opposite corner to define the window dimensions.

[Edit >]

- **[Edit >] Single** is used to edit one or more grid cells belonging to the same group of boundary condition cells.
- **[Edit >] Group** is used to edit all of the grid cells belonging to the selected group of boundary condition cells.
- **[Edit >] Property** is used to edit the parameter values associated with a boundary condition zone

[Copy >]

- **[Copy >] Single** is used to select the boundary grid cell to copy and then select the destination grid cells where it will be copied.
- **[Copy >] Layer** is used to copy all of the boundary data from a selected boundary group to one or more selected model layers.
- **[Copy >] Row** is used to copy all of the boundary data from a selected boundary group to one or more selected model rows.
- **[Copy >] Column** is used to copy all of the boundary data from a selected boundary group to one or more selected model columns.

[Erase >]

- **[Erase >] Single** is used to select individual grid cells where the boundary condition will be erased (deleted). Hold the mouse button down to select multiple grid cells, or click the right mouse button to unselect grid cells.
- **[Erase >] Polygon** is used to digitize a polygon around the group of grid cells where the boundary condition will be erased (deleted). Left-click at the start point of the polygon to begin digitizing the shape of the polygon and right-click near the start point to close the polygon.
- **[Erase >] Group** is used to erase (delete) all of the grid cells belonging to the selected group of boundary condition cells.

3.5.2 Flow Boundary Conditions

Visual MODFLOW supports the following groundwater flow boundary conditions types:

- **Constant Head (CHD)** - see page 117
- **River (RIV)** - see page 119
- **General-Head (GHB)** - see page 128
- **Drain (DRN)** - see page 131
- **Wall (HFB)** - see page 134
- **Stream (STR)** - see page 122
- **Recharge (RCH)** - see page 136
- **Evapotranspiration (EVT)** - see page 139

The following sections provide a description of the data requirements for each of these boundary condition types, and the options for assigning, editing and importing the required data.

Steady-State vs. Transient Flow Boundary Conditions

For transient simulations, MODFLOW requires the time element of the boundary conditions to be defined using Stress Period “counters” as opposed to using “real” times. As a result each time interval for a transient model must be pre-defined in terms of Stress Period before any boundary condition data is defined. Unfortunately, accommodating this format is quite tedious because the data collected for rainfall and groundwater recharge doesn’t always follow the same time schedules as data collected for other boundary conditions like well pumping rates and surface water levels. This approach also makes it difficult to utilize raw field data collected and recorded in terms of real times.

In Visual MODFLOW, a Time Period is similar to a Stress Period, but with two important exceptions:

- A Time Period is defined using real times and real time unit, and
- Each boundary condition grid cell may contain different Time Periods

The advantage of this approach is the ability to clearly see the magnitude of time for each Time Period (as opposed to interpreting data such as “from Stress Period 1 to Stress Period 2”).

Each group of boundary condition grid cells requires a minimum of one Time Period of data containing a **Start Time**, a **Stop Time** and a complete set of data for the selected boundary condition type (the required data for each boundary condition type are described later in this section). For steady-state simulations, Visual MODFLOW requires data for only a single Time Period, while for transient simulations Visual MODFLOW can accommodate an unlimited number of Time Periods.

For steady-state simulations the **Stop Time** value is irrelevant because the term “steady-state” implies the model results are not changing with time. Therefore, a **Stop**

Time value of 1 time unit is commonly used. However, if the model may be used to evaluate a transient simulation in the future, it is probably a better idea to give it a more realistic value corresponding to the potential time frame of interest.

If a steady-state simulation is run using a model containing transient boundary condition data, only the data from the first Time Period of each grid cell will be used for the steady-state conditions.

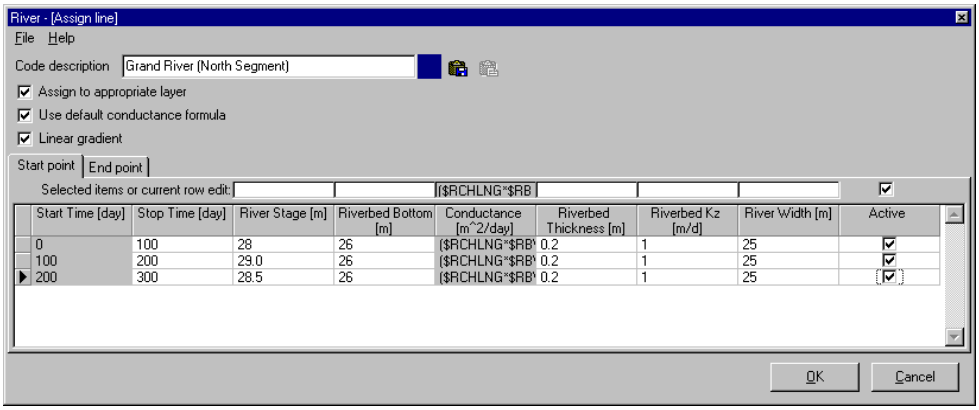
If a transient model is run for 10 years, and one of the boundary conditions is defined only for a period up to 7 years, Visual MODFLOW will assume this boundary condition does not exist for the remaining 3 years of the simulation.

> **Note:** For a steady-state simulation, a minimum of one active grid cell in the model MUST contain a head-dependent boundary condition type. Otherwise, the model is indeterminate and the solution will not converge. This head-dependent boundary condition acts as a reference head for all calculations. The head-dependent boundary condition type can be one of the following:
>
> - Constant Head (CHD)
> - River (RIV)
> - Stream (STR)
> - General-Head (GHB)
> - Reservoir (RSV)
> - Lake (LAK)
>
> For a transient simulation the specified initial heads are sufficient for a determinant solution.

Assigning Flow Boundary Conditions

One of the most significant improvements in Visual MODFLOW v.3.0 is the enhanced data input and editing options available for assigning and editing Constant Head, River, Drain, General-Head and Stream boundary conditions. Although each of these boundary condition types requires different sets of parameters, the data input windows each have similar features and functionality as shown in the following figure and described below.

For the purposes of this document, an example of assigning a River boundary condition will be used to describe the features and functionality of the new data input and editing options.



The above figure is used to enter data for a River boundary condition using the **[Assign >] Line** option.

Code description

The **Code description** is an alphanumeric description for the selected group of model grid cells. This **Code description** is used to identify this group of grid cells for the purpose of editing the boundary condition attributes for the entire group of cells at a later time (see section Editing Flow Boundary Conditions on page 113).

Assign to appropriate layer

The **Assign to appropriate layer** option is used to automatically assign the boundary condition from the selected grid cell to the grid cell in the 'appropriate' layer, where the appropriate grid cell is located in the layer corresponding to the head-related value assigned to the selected grid cell.

For Constant Head, River and Stream boundary conditions, MODFLOW does not allow the head-related values (Head, River Stage and Stream Stage, respectively) to be less than the bottom elevation of the grid cell in which this boundary condition is assigned. If the head-related value assigned to the selected grid cell is lower than the grid cell bottom elevation, this option will essentially 'push' the boundary condition down from the selected grid cell to the next lowest grid cell where the head-related value is not below the grid cell bottom elevation.

Consider a model with the following dimensions:

- 0 - 1000 m in the X-Direction
- 0 – 1000 m in the Y-Direction
- 0 – 100 m in the Z-Direction
- 10 rows x 10 columns x 5 layers

If a **Constant Head** boundary condition of 70 m is assigned along the west boundary in Layer 1, Visual MODFLOW will not accept it because 70 m is below the bottom elevation of Layer 1. However, if the **Assign to appropriate layer** option is selected,

Visual MODFLOW will accept this data and assign a **Constant Head** boundary condition along the west boundary of Layer 2.

Use default conductance formula

The **Use default conductance formula** option is used to calculate the Conductance value for River, Stream, Drain and General Head boundary conditions using a mathematical expression containing array variables (see section Using Mathematical Formulas and Array Variables on page 108). If the **Use default conductance formula** option is selected (as shown in the above figure) the conductance value will be calculated using a default formula associated with each boundary condition type. If the **Use default conductance formula** option is not selected, a conductance value will need to be entered directly.

The advantage of using the default conductance formula to calculate the conductance values for the group of grid cells is that each grid cell will be assigned a conductance value proportional to the size of the grid cell.

> **Note:** If the **[Assign >] Line** option is used to select the grid cells then the default conductance formula will use the length of the line passing through each cell to calculate the conductance. If the **[Assign >] Single** or **[Assign >] Polygon** options are used to select the grid cells then the default conductance formula will use the cell dimensions to calculate the conductance.

Linear gradient

The **Linear gradient** option is only available when **[Assign > Line]** is used to select the boundary condition grid cells. If **Linear gradient** option is not selected, then the **Assign Line** data entry window will require a single set of attributes to be assigned to each grid cell intersected by the line. If the **Linear gradient** option is selected (as shown in the above figure) then the **Assign Line** dialog will prompt for two sets of boundary condition data; one set for the grid cell at the **Start Point** of the line, and one set for the grid cell at the **End Point** of the line. The boundary condition data for the grid cells between the **Start Point** grid cell and the **End Point** grid cell will be linearly interpolated between these two points using the formula below.

$$\$X_i = \$X_{SP} + (\$X_{SP} - \$X_{EP}) \times \frac{\$TVAR_{1,i}}{\$LENGTH}$$

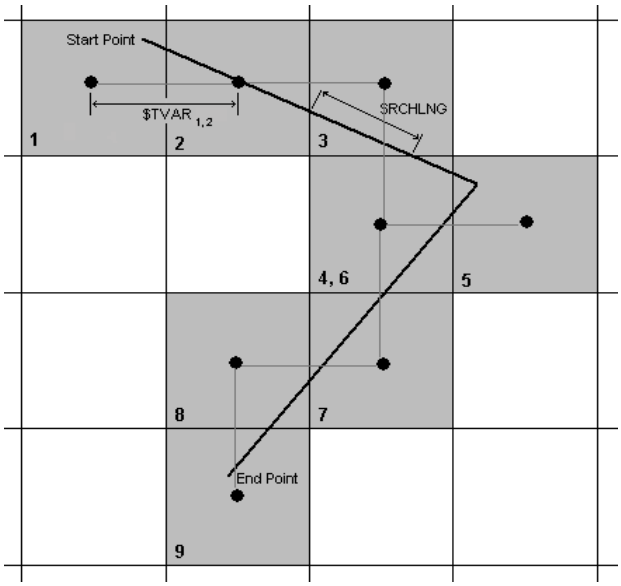
Where:

$\$X_i$	is the boundary condition parameter value at the ith grid cell along the line
$\$X_{SP}$	is the boundary condition parameter value at the **Start Point** of the line
$\$X_{EP}$	is the boundary condition parameter value at the **End Point** of the line

$TVAR$_{1, i}$ is cumulative length of the line at the i^{th} grid cell along the line as measured from the centre of the **Start Point** grid cell through the centre of each successive grid cell along the line (see figure below).

$LENGTH is the total length of the line as measure from the centre of the **Start Point** grid cell through to the centre of the **End Point** grid cell (see figure below).

When the line is digitized from the **Start Point** to the **End Point**, each grid cell is numbered in sequence according to the order in which the line passes through each cell. If the line passes through the same grid cell twice, the grid cell will be numbered twice as seen for grid cell 4, 6 in the figure below. As a result, the parameter value calculated for grid cell #6 will over-write the parameter value calculated for grid cell #4.



Entering Flow Boundary Condition Data

The features and functionality of boundary condition data entry tables are similar to what would be expected of a typical data entry table. For example:

<Tab>	advances to the next field on the right
<Shift><Tab>	advances to the next field on the left
<Down Arrow>	moves the cursor down one row to the next time period
<Up Arrow>	moves the cursor up one row to the previous time period

However, the data entry tables have some special features for making it easier and faster to enter repetitive data, import data from external files, and assign data using formulas and array variables.

Adding a Time Period

A new time period can be added using three different keys:

<Tab>	If the cursor is in the last column of a row, pressing the **<Tab>** key will create a new empty time period and the cursor will be active in the **Stop Time** field.
<Down Arrow>	If the cursor is in the last time period, pressing the **<Down Arrow>** will create a new time period and copy all attributes from the previous time period.
<Enter>	If the cursor is in the last time period, pressing the **<Enter>** key will create a new empty time period

Deleting a Time Period

Unwanted time periods can be deleted by clicking the right mouse button in the **Stop Time** field of the time period and choosing the **Delete time period** option

Inserting a Time Period

A time period can be inserted into an existing schedule by clicking the right mouse button in the **Stop Time** field of the time period immediately following the time to be inserted and selecting the **Insert time period** option.

Copying Repetitive Data

In many cases with transient simulations there will only be a single parameter of each boundary condition type that changes with time (usually the head-related parameter). For example, with a River boundary, the **River Stage Elevation** value will change with time, but the **River Bottom Elevation** and the **Conductance** are usually static regardless of the season. However, MODFLOW requires that each attribute of a boundary condition must be defined for each time period. In order to make this situation more convenient, the data from the current time period can be copied to a new time period by pressing the **<Down Arrow>** key to create a new time period. Alternatively, pressing the **<Tab>** key in an empty field of the new time period will automatically copy the attribute value from the previous time period.

The Formula Bar

The **Formula Bar** is the row of input fields located directly above the column headers of each boundary condition parameter. Although these fields can be used to enter parameter values for a single time period, the primary purpose of the **Formula Bar** is assign parameter values for multiple time periods. For example, clicking the column header of a boundary condition parameter will select the entire column of data values (i.e. all time periods) and will enable the Formula field for the selected parameter. Any

value entered in the Formula field will be applied to all time periods for the selected parameter (similar to how a spreadsheet works).

Using Mathematical Formulas and Array Variables

Although most boundary condition parameters are defined using real numbers, there are many situations where parameters are better defined using a mathematical formula containing array variables. An array variable is a model parameter that is defined for each model grid cell and may (or may not) change from cell to cell. Each array variable is identified by a "$" prefix on the variable name. An example of an array variable is the bottom elevation of each grid cell (**$BOT**).

The expression interpreter used by Visual MODFLOW is capable of handling most basic mathematical expressions using generally accepted standards as follows:

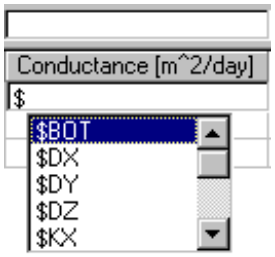
* denotes a multiplication sign

/ denotes a division sign

+ denotes an addition sign

- denotes a minus sign

The list of array variables for each boundary condition parameter can be seen by simply clicking in the parameter field and typing "$" as shown in the following figure. Use the mouse pointer to select the desired variable or simply type the variable name.



> **Note:** If a variable name is manually entered without the "$" prefix, it will not be recognized by Visual MODFLOW and a "Syntax error" message will be issued upon trying to close the data entry dialog.

The array variables available for creating mathematical expressions are as follows:

$BOT	Bottom elevation of grid cell [L]
$DX	Length of grid cell in X-direction [L]
$DY	Length of grid cell in Y-direction [L]
$DZ	Length (thickness) of grid cell in Z-direction (in units of length)
$KX	Hydraulic conductivity in the X-direction (in units of length per time)
$KY	Hydraulic conductivity in the Y-direction (in units of length per time)
$KZ	Hydraulic conductivity in the Z-direction (in units of length per time)
$MBOT	Model bottom elevation for the X-Y location of the grid cell (in units of length)

$UCTOCOND Unit conversion factor for converting the length and time units used for hydraulic conductivity to the length and time units used for Conductance

$**RCHLNG** Length of line passing through each grid cell (in units of length)*

$LENGTH Total length of the line as measured through the centre of each grid cell (in units of length)*

$TVAR Cumulative length of line as measured through the center of each grid cell (in units of length)*

* **$RCHLNG**, **$LENGTH** and **$TVAR** variables are only available when the [**Assign >] Line** option has been used to select the grid cells.

Additional array variables are available for specific boundary condition types depending on the parameters required.

A common example of where a mathematical expression containing array variables is very useful is for defining the Conductance values for grid cells containing a River boundary condition (see section section River (RIV) Boundary Conditions on page 119). In this example, the Conductance for the River boundary condition in each grid cell is calculated using the following formula:

$$\$COND = \left(\frac{\$RCHLNG \times \$RBWIDTH \times \$K}{\$RBTHICK}\right) \times \$UCTOCOND$$

Where, **$COND** = Riverbed Conductance [L^2/T]

$RCHLNG = Reach length of the river in each grid cell [L]

$RBWIDTH = Riverbed width in each grid cell [L]

$RBTHICK = Riverbed thickness in each grid cell [L]

$K = Riverbed vertical hydraulic conductivity [L/T]

$UCTOCOND = Unit conversion factor

The reach length (**$RCHLNG**) of the river in each grid cell is determined from the line used to digitize the river location in the model (only available when the **[Assign > Line]** option is used). The riverbed width (**$RBWIDTH**), riverbed thickness (**$RBTHICK**) and riverbed hydraulic conductivity (**$K**) are user-defined parameters. The unit conversion factor (**$UCTOCOND**) is used to convert the hydraulic conductivity value from conductivity units to conductance units.

This type of mathematical expression can be used to define virtually any boundary condition parameter by simply entering the expression in the data input field.

Visual MODFLOW has several default formulas for calculating the conductance values for each boundary condition type. These formulas are described in the sections describing each boundary condition type.

Importing Transient Boundary Condition Data

If a simulation has many time periods, the process of manually entering the data for each time period can be time consuming and cumbersome, particularly if the data is already saved in electronic format. For these situations, Visual MODFLOW includes a versatile data import utility for each MODFLOW boundary condition type.

In order to accommodate the raw data formats typically encountered by groundwater modelers, Visual MODFLOW does not required the imported data file to contain all of the parameters for the selected boundary condition type, but rather, only the time and value for the transient parameter(s) as shown in the following table. This eliminates the need for any spreadsheet manipulations of the data to "fit" the data format required by MODFLOW.

Visual MODFLOW supports two different time formats:

- **Relative time** is used when all imported data is reported in relative time unit values starting from time zero (see example in table below)
- **Date and time** is used when all imported data is reported in real date and time units (see example in table below)

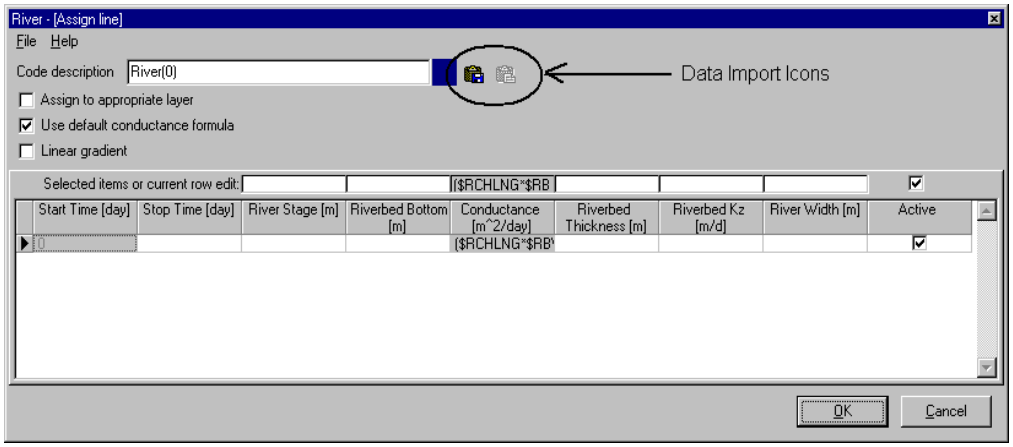
Example Time Format Data

Relative Time Data		Date and Time Data		
Time (days)	River Stage (m amsl)	Date (dd/mm/yy)	Time hh:mm:ss	River Stage (m amsl)
0	18.2	01/01/98	15:10:00	18.2
30	18.5	01/02/98	15:10:00	18.5
60	18.6	01/03/98	15:10:00	18.6
90	18.8	01/04/98	15:10:00	18.8
120	18.6	01/05/98	15:10:00	18.6
150	18.2	01/06/98	15:10:00	18.2
180	17.8	01/07/98	15:10:00	17.8

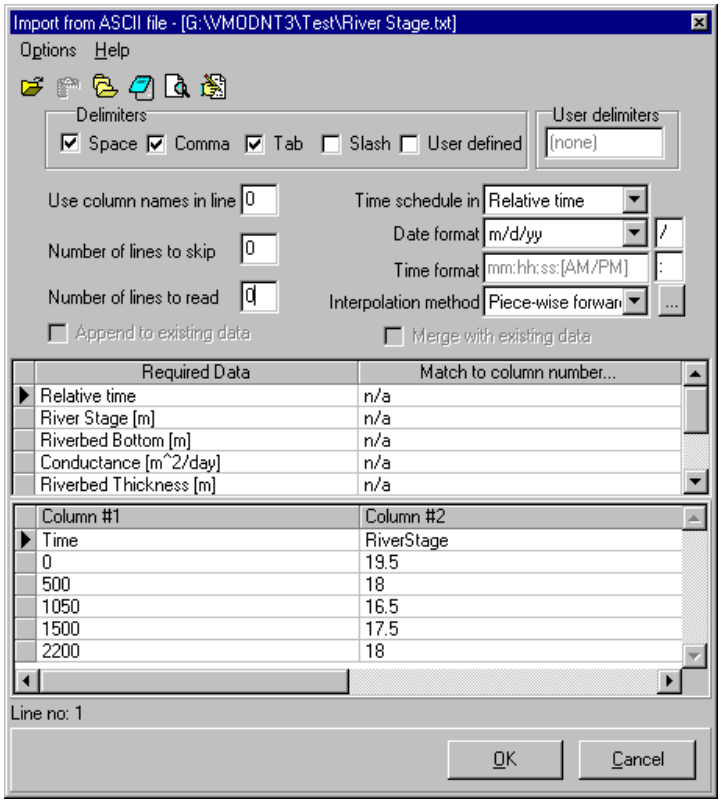
Note: The date for the imported data need to later than the **Starting Date** for the model. The **Starting Date** for the model can be viewed and/or modified by returning to the **Main Menu** and selecting **File/Model Settings**.

The steps required to import transient boundary condition data are described below. The example screen captures were generated using the **[Assign > Line]** operation to assign a **River** boundary condition.

.



Click the **Import from ASCII file** icon to import transient boundary condition data saved in an external file. An **Open** file dialog will appear to select the ASCII text (.TXT) file containing he boundary condition data. Once the data file is selected, the following **Import** window will appear, or



Note: The **Import from ASCII file** window shown above has the same functionality as the **Import from Clipboard** option.

The **Options** menu list six different options corresponding to the icons listed in the toolbar:

Load new data file	Load a different ASCII data file
Paste data from clipboard	Replace the existing data with data from the Windows clipboard (only active if clipboard contains data)
Reload source data file	Reload the source data file after changes have been made
Edit source data file	Open and edit the source data file
Preview imported data	Previews the imported data set as it will appear in the boundary condition data entry table
Preview data file	Previews the data being imported in the data preview table

The **Delimiters** frame provides a selection of common delimiters used to separate different data values in the same row. If the required delimiter is not available in the pre-defined delimiters, a **User-defined** delimiter can be entered.

The **Use column headers in line** field is used to identify which line of the data file contains the titles (header) for each column of data. The default setting is “0”.

The **Number of lines to skip** field is used to identify the number of lines of data to skip. This is used if some redundant or unreliable data occurs at the start of the data file. The default setting is “0”, indicating that the first line of the data file will be read.

The **Number of lines to read** field is used to identify how many lines of data will be imported. This is used if some redundant or unreliable data occurs at the end of the data file. The default setting is “0” indicating that all data after the starting point will be imported.

The **Time schedule in** field contains a selection of two time formats:

- **Relative time** is used when all imported data is reported in relative time unit values starting from time zero (see example in table below)
- **Date and time** is used when all imported data is reported in real date and time units (see example in table below)

The **Date format** field is used to select the appropriate date format for the ASCII data file. This field is only available when **Date and Time** are selected in the **Time Schedule** field.

The **Time format** field is used to select the appropriate time format for the ASCII data file. This field is only available when **Date and Time** are selected in the **Time Schedule** field.

The **Interpolation method** field is used to select the appropriate interpolation method to use for creating the time schedules containing **Start Time** and **Stop Time** for each time period. The time interpolation method selected will determine how the data from the data files are manipulated to fit the required format. There are four time interpolation methods available:

- **Piece-wise backward**
- **Piece-wise middle**
- **Piece-wise forward**
- **Interpolated** (only available for Constant Head boundary condition)

The **Browse [...]** button shows a graphical description of each interpolation method and how the raw data is interpreted and manipulated by Visual MODFLOW to fit the required time period format.

The **Required Data** column lists the parameters required by the selected boundary condition type. In the example above, the **Required Data** column lists the parameters required by the **River** boundary condition.

The **Match in column number** column is used to match the **Required Data** fields to the columns of data from the ASCII text file. In the example above, the ASCII text file contained only two columns of data; (1) Time, and: (2) River Stage. As a result, **Column #1** is matched to the **Relative time** field and **Column #2** is matched to the **River Stage** field as shown in the following figure. The remaining **Required Data** fields may be left as “n/a” (not available) or as blank entries and are not assigned any values during the data import process.

Editing Flow Boundary Conditions

Existing boundary condition data can be modified by selecting either **[Edit > Single]**, or **[Edit > Group]** from the toolbar on the left-hand side of the Visual MODFLOW window.

- The **[Edit > Single]** option can be used to select one or more grid cells belonging to the same group of boundary condition cells.
- The **[Edit > Group]** option can be used to select all of the grid cells belonging to the selected group of boundary condition cells.

Once the desired grid cells are selected, a **Boundary Condition - Edit** window will appear as shown in the following figure. This dialog will have different parameters depending on the selected boundary condition type, but the functionality of this window is similar for most MODFLOW boundary conditions.

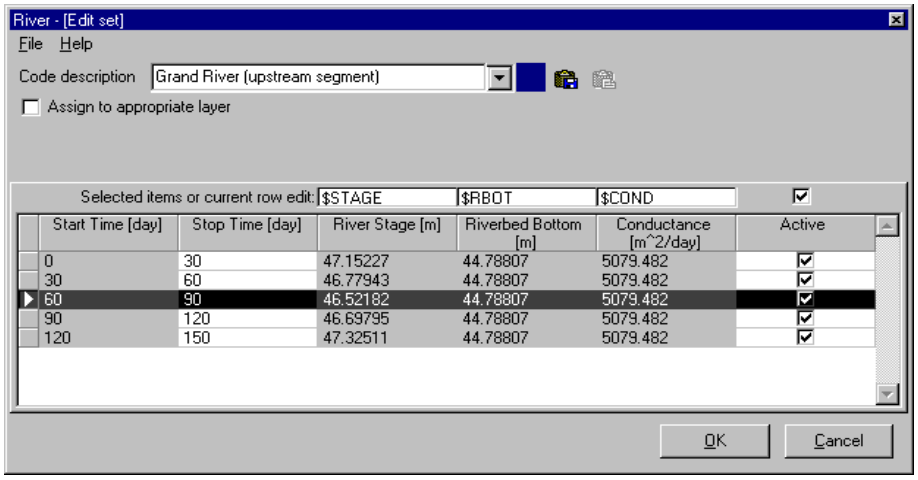
The **Boundary Condition - Edit** window has a very similar appearance and much of the same functionality as the **[Boundary Condition] - Assign** window, but there are some important differences to be aware of:

- The parameter value entry fields in the table are disabled, meaning that no values can be entered directly into these fields

- The **[Boundary Condition] - Edit** window contains only MODFLOW-related parameters
- The parameter fields may contain ranges of values

Note: The reason for these differences is explained at the end of this section, but will likely become apparent as the functionality of this window is explained.

The **[Boundary Condition] - Edit** window can be used to insert or delete time periods, and to add, subtract, divide or multiply parameter values for one time period, multiple time periods, or all time periods.



Modifying Parameter Values

To modify a boundary condition parameter value, simply click the mouse pointer on the target time period and the **Formula Bar** above each column will be activated. Each Formula field contains a variable name corresponding to the boundary condition parameter for each column. This parameter variable represents the parameter value(s) for the selected time period(s). This parameter value(s) may be modified by either:

- Option (1): Replacing the parameter value(s) for the selected time period(s) with a constant value, or
- Option (2): Performing a mathematical operation on the variable to uniformly increase or decrease the parameter value for the selected time period(s)

For Option (1) simply replace the variable name with a numeric value and press <Enter>. Be careful when using this option because it will replace a range of values for all selected grid cells in the boundary group with a constant value. For example, a line of River boundary cells may have a **River Stage Elevation** ranging from 100 to 95 ft amsl. If the **$STAGE** variable is replaced by a numeric value of 101, then all River boundary cells along this line will have a **River Stage Elevation** of 101 ft amsl.

For Option (2) a mathematical operation (addition, subtraction, multiplication and division) may applied to the variable to affect the value as desired. For example:

- The **River Stage** can be increased by a uniform value of 2.5 in all selected grid cells belonging to the boundary group by entering "**$STAGE+2.5**" in the **Formula Bar** and pressing the **<Enter>** key.
- The **River Stage** can be multiplied by a uniform value of 1.1 in all selected grid cells belonging to the boundary group by entering "**$STAGE*1.1**" in the **Formula Bar** and pressing the **<Enter>** key.
- The **River Stage** can be decreased by a uniform value of 1.5 in all selected grid cells belonging to the boundary group by entering "**$STAGE-1.5**" in the **Formula Bar** and pressing the **<Enter>** key.
- The **River Stage** can be divided by a uniform value of 1.2 in all selected grid cells belonging to the boundary group by entering "**$STAGE/1.2**" in the **Formula Bar** and pressing the **<Enter>** key.

Additional array variables are also available for including in the parameter expressions and can be viewed by simply typing "**$**" in the formula field. For example the **River Stage** may be set equal to 1.0 ft below the top of the grid cell elevation in all grid cells by entering the following expression in the **River Stage** formula cell.

$BOT+$DZ-1.0

where:

$BOT is the elevation of the bottom of the grid cell, and

$DZ is the length of the grid cell in the Z-direction

Selecting Time Periods

To select the time period of interest simply click the mouse pointer on the time period containing the parameter value(s) that need to be modified. To simultaneously modify multiple time period, click on the left-most column of the starting time period and drag the mouse to the ending time period, or hold down the **<Ctrl>** key and click on individual time periods. To simultaneously modify a parameter for all time periods, click the mouse pointer in the column header of the parameter.

Inserting a Time Period

To insert a time period in the time schedule, right click the mouse pointer in the time period that should be sub-divided and select the **Insert row** option. A new time period will be created containing the data from the previous time period and with a blank **Stop Time** value. The **Stop Time** value entered will be automatically copied to the **Start Time** of the following time period.

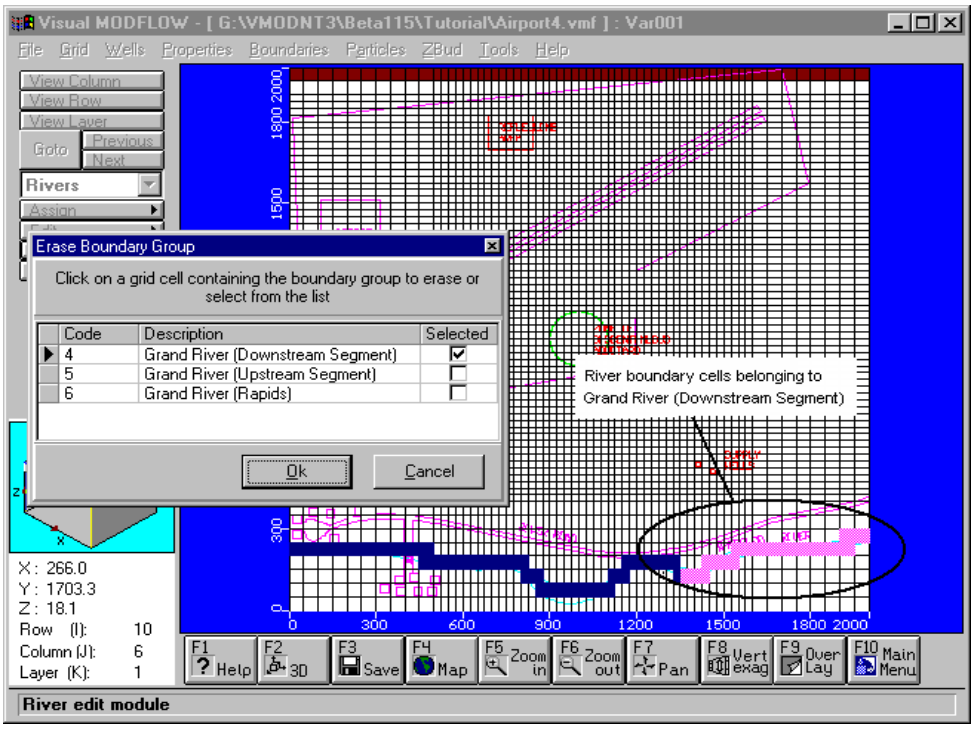
Deleting a Time Period

To delete a time period from the time schedule, right-click the mouse pointer in the time period that should be removed and choose the **Delete selected row(s)** option. The selected time period and the associated data will be deleted from the time schedule and the **Start Time** from the following time period will automatically be adjusted to match the **Stop Time** from the prior time period.

Erasing Flow Boundary Conditions

Boundary conditions can be erased (deleted) from the model by selecting one of the **[Erase >]** options from the left-hand toolbar.

- **[Erase >] Single** is used to click the mouse pointer on individual boundary grid cells to erase, or to click-and-drag the mouse pointer across multiple boundary grid cells.
- **[Erase >] Polygon** is used to digitize a polygon around the cells to erase. Left-click at the start point of the polygon to begin digitizing the shape of the polygon and right-click near the start point to close the polygon.
- **[Erase >] Group** can be used to select a boundary group from a list of available boundary groups (as shown in the following figure), or it can be used to click the mouse pointer on a boundary grid cell in order to select the entire boundary group.



Copying Flow Boundary Conditions

Boundary condition data can be copied from one grid cell to another grid cell using one of the **[Copy >]** options from the left-hand toolbar.

- **[Copy >] Single** is used to select the boundary grid cell to copy and then select the destination grid cells where it will be copied.

- **[Copy >] Layer** is used to copy all of the boundary data from a selected boundary group to one or more selected model layers.
- **[Copy >] Row** is used to copy all of the boundary data from a selected boundary group to one or more selected model rows.
- **[Copy >] Column** is used to copy all of the boundary data from a selected boundary group to one or more selected model columns.

Constant Head (CHD) Boundary Conditions

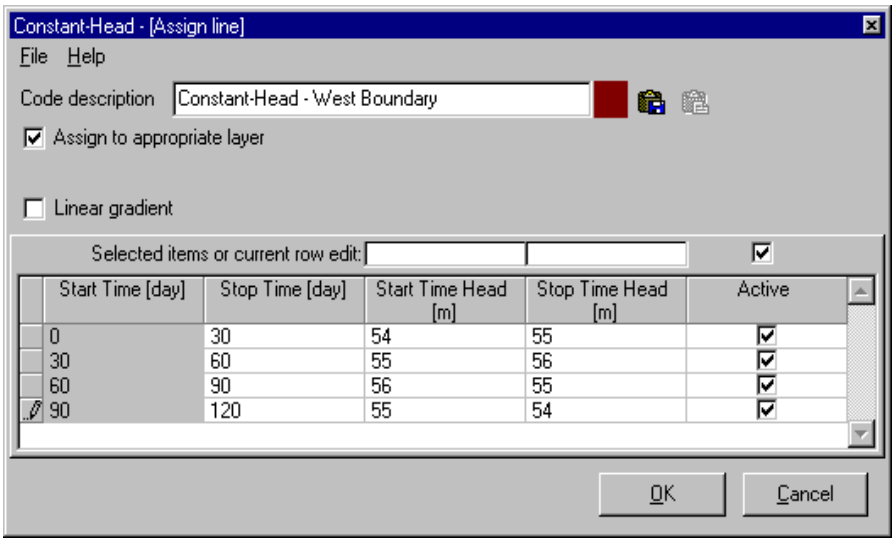
Visual MODFLOW supports the Time-Variant Specified-Head Package included with MODFLOW. The Visual MODFLOW input data for Constant Head grid cells is stored in the *projectname*.VMB file (see Appendix A), while the MODFLOW input data for Constant Head grid cells is stored in the *projectname*.CHD file (see MODFLOW-2000 Reference Manual .PDF file provided with the Visual MODFLOW installation CD-ROM).

The Constant Head boundary condition is used to fix the head value in selected grid cell regardless of the system conditions in the surrounding grid cells, thus acting as an infinite source of water entering the system, or as an infinite sink for water leaving the system. As such, Constant Head boundary conditions can have a significant influence on the results of a simulation and may lead to unrealistic predictions, particularly when used in locations which are close to the area of interest.

Unlike most other transient MODFLOW boundary condition packages, the CHD package allow the specified heads to be linearly interpolated in time between the beginning and end of each stress period, such that the specified head for a grid cell may change at each time step of a given stress period. The CHD package requires the following information for each Constant Head grid cell for each stress period:

- **Start Head:** Specified head value at the beginning of the stress period
- **Stop Time:** Specified head value at the end of the stress period

Constant Head boundary conditions can be assigned by selecting **Boundaries/ Constant Head (CHD)** from the **Input** section of Visual MODFLOW and using any of the **[Assign >]** options from the left-hand toolbar (described in the section Tools for Assigning and Editing Boundary Conditions on page 100). Once the model grid cells are selected, a data input window will appear as shown in the following figure.



The **Code description** is described on page 104.

The **Assign to appropriate layer** option is described on page 104.

The **Linear gradient** option is described on page 105.

The **Constant Head** data required by Visual MODFLOW is identical to the information required by the CHD input file described above:

- **Start Time Head** is the specified head value at the start of the time period (**$SHEAD**).
- **Stop Time Head** is the specified head value at the end of the time period (**$EHEAD**).

When multiple time steps are being assigned, Visual MODFLOW will automatically copy the **Stop Time Head** from the previous time period to the **Start Time Head** of the new time period.

For details on entering boundary condition data refer to the section Entering Flow Boundary Condition Data on page 106.

For details on using mathematical formulas and array variables to define boundary condition data refer to the section Using Mathematical Formulas and Array Variables on page 108.

For details on importing transient boundary condition data refer to the section Importing Transient Boundary Condition Data on page 110.

For details on editing boundary conditions data refer to the section Editing Flow Boundary Conditions on page 113.

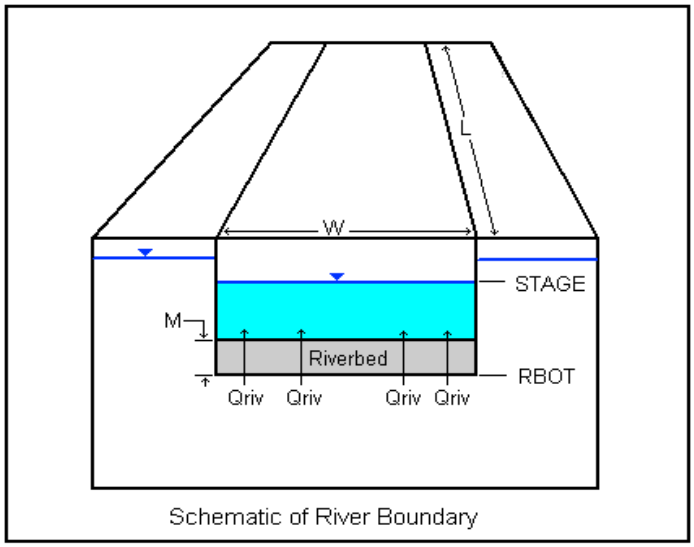
For details on erasing boundary conditions refer to the section Erasing Flow Boundary Conditions on page 116.

For details on copying boundary condition data refer to the section Copying Flow Boundary Conditions on page 116.

River (RIV) Boundary Conditions

Visual MODFLOW supports the River Package included with MODFLOW. The Visual MODFLOW input data for River grid cells is stored in the *projectname*.VMB file (see Appendix A), while the MODFLOW input data for River grid cells is stored in the *projectname*.RIV file (see MODFLOW-2000 Reference Manual .PDF file provided with the Visual MODFLOW installation CD-ROM).

The River boundary condition is used to simulate the influence of a surface water body on the groundwater flow. Surface water bodies such as rivers, streams, lakes and swamps may either contribute water to the groundwater system, or act as groundwater discharge zones depending on the gradient between the surface water body and the groundwater system. The MODFLOW River Package *(projectname*.RIV) simulates the surface water / groundwater interaction via a seepage layer separating the surface water body from the groundwater system (see figure below).



Schematic of River Boundary

The MODFLOW River Package input file (*projectname*.RIV) requires the following information for each grid cell containing a River boundary;

- **River Stage:** The free water surface elevation of the surface water body. This elevation may change with time.
- **Riverbed Bottom:** The elevation of the bottom of the seepage layer (bedding

material) for the surface water body.

- **Conductance:** A numerical parameter representing the resistance to flow between the surface water body and the groundwater caused by the seepage layer (riverbed).

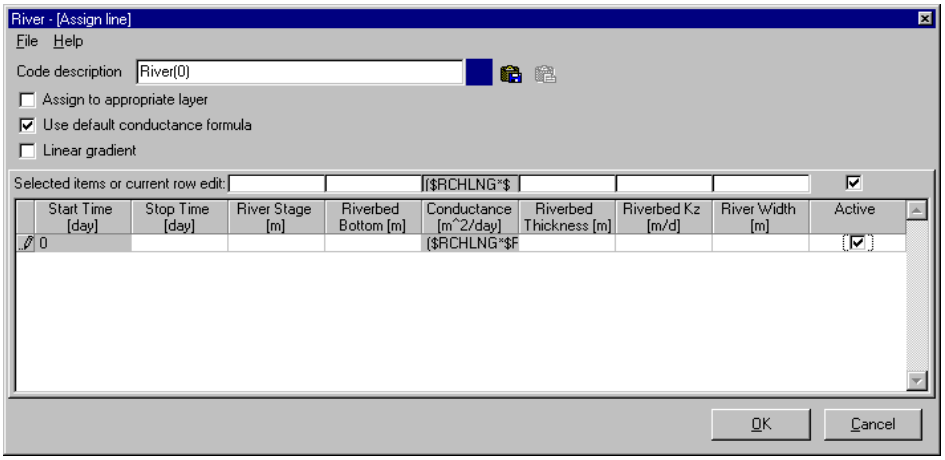
The Conductance value (C) may be calculated from the length of a reach (L) through a cell, the width of the river (W) in the cell, the thickness of a river bed (M), and the vertical hydraulic conductivity of the river bed material (K) using the following formula.

$$C = \frac{K \times L \times W}{M}$$

For situations where the River package is used to simulate lakes or wetlands, the L and W variables would correspond to the X-Y dimension of the River boundary grid cells.

River boundary conditions can be assigned by selecting **Boundaries/River (RIV)** from the **Input** section and using any of the **[Assign >]** options from the left-hand toolbar (described in the section Tools for Assigning and Editing Boundary Conditions on page 100).

Once the model grid cells are selected, a data input window will appear as shown in the following figure and described below.



The **Code description** is described on page 104.

The **Assign to appropriate layer** option is described on page 104.

The U**se default conductance formula** option is described on page 105.

The **Linear gradient** option is described on page 105.

When a River boundary condition is assigned, the **Use default conductance formula** option is automatically selected.

If the **Use default conductance formula** option is selected, the River boundary condition requires the following data:

- **River Stage**: The free water surface elevation of the surface water body.
- **Riverbed Bottom**: The elevation of the bottom of the seepage layer (bedding material) for the surface water body.
- **Conductance**: A numerical parameter representing the resistance to flow between the surface water body and the aquifer (this field is read-only and is calculated using the formula described below).
- **Riverbed Thickness**: Thickness of the riverbed (seepage layer).
- **Riverbed Kz**: Vertical hydraulic conductivity of the riverbed material.
- **River Width**: Width of the river.

If the grid cells were selected using the **[Assign >] Line** option, the default conductance formula is as follows:

$$\$COND = \frac{\$RCHLNG \times \$WIDTH \times \$K \times \$UCTOCOND}{\$RBTHICK}$$

If the grid cells were selected using **[Assign >] Single, [Assign >] Polygon**, or **[Assign >] Window**, the default conductance formula is as follows:

$$\$COND = \frac{\$DX \times \$DY \times \$K \times \$UCTOCOND}{\$RBTHICK}$$

Where:

$COND	is the **Conductance**
$RCHLNG	is the reach length of the river line in each grid cell
$WIDTH	is the **River Width** in each grid cell
$K	is the **Riverbed Kz**
$UCTOCOND	is the conversion factor for converting the **$K** value to the same L and T units used by **$COND**
$RBTHICK	is the **Riverbed Thickness**
$DX	is the length of each grid cell in the X-direction
$DY	is the length of each grid cell in the Y-direction

If the **Use default conductance formula** option is turned off, the fields used for calculating the River Conductance value (**River Width**, **Riverbed Thickness**, and

Riverbed Kz) are removed from the table and the **Conductance** field becomes a read/write field where any value or alternate formula may be entered.

> **Note:** When Conductance values (or any other parameters) are calculated using a formula, the array variables and formulas are not saved together with the River boundary data and cannot be recalled or modified at a later time. Visual MODFLOW only stores the **River Stage**, **River Bottom** and **Conductance** values for each grid cell.

For details on entering boundary condition data refer to the section Entering Flow Boundary Condition Data on page 106.

For details on using mathematical formulas and array variable to define boundary condition data refer to the section Using Mathematical Formulas and Array Variables on page 108.

For details on importing transient boundary condition data refer to the section Importing Transient Boundary Condition Data on page 110.

For details on editing boundary conditions data refer to the section Editing Flow Boundary Conditions on page 113.

For details on erasing boundary conditions refer to the section Erasing Flow Boundary Conditions on page 116.

For details on copying boundary condition data refer to the section Copying Flow Boundary Conditions on page 116.

Stream (STR) Boundary Conditions

Visual MODFLOW supports the Streamflow-Routing Package STR1 (Prudic, 1989) included with MODFLOW. The MODFLOW input data for Stream grid cells is stored in the *projectname*.STR file (see MODFLOW-2000 Reference Manual .PDF file provided with the Visual MODFLOW installation CD-ROM).

The function of the Streamflow-Routing Package is to account for the amount of flow in stream and to simulate the interaction between surface streams and groundwater. Streams are divided into segments and reaches. Each reach corresponds to individual grid cells, while segments consist of a group of grid cells connected in downstream order. Streamflow is accounted for by specifying a stream inflow for the first reach in each segment, and then calculating the streamflow to adjacent downstream reaches in each segment as equal to inflow in the upstream reach plus/minus leakage from/to the aquifer in the upstream reach.

Streamflows into a segment that is formed from tributary streams is calculated by adding the outflows from the last reach in each of the specified tributary segments. If a segment is a diversion, then the specified flow into the first reach of the diversion segment is subtracted from the flow in the main stream. However, if the specified flow of the diversion is greater than the flow in the main stream, then no flow is diverted.

The Streamflow-Routing Package requires the following information for each reach of the Stream (each Stream grid cell):

- **Stream Inflow:** Inflow rate to the first reach of a stream segment, in units of length cubed per time. Use a value of -1 to indicate the Stream Inflow will be calculated using the outflow from the last reach(es) of the upstream segment(s).
- **Stream Stage:** The free water surface elevation of the surface water body.
- **Streambed Top:** The elevation of the top of the seepage layer (bedding material) for the surface water body.
- **Streambed Bottom:** The elevation of the bottom of the seepage layer (bedding material) for the surface water body.
- **Conductance:** A numerical parameter representing the resistance to flow between the surface water body and the groundwater caused by the seepage layer (riverbed).
- **Width:** The width of the stream channel in units of length.
- **Slope:** The slope of the stream channel in units of length per length.
- **Roughness:** Manning's roughness coefficient for the stream channel.

The Width, Slope and Roughness values are not required unless the Stream Stage is being calculated using Manning's equation for open channel flow (Ozbilgin and Dickerman, 1984). If the Stream Stage is being calculated then the specific Stream Stage value is ignored.

> **Note:** The method for specifying the Stream Stage value is a global setting. The Stream Stage must either be specified for ALL reaches in ALL Segments, or it must be calculated for ALL reaches in ALL segments. The Stream Stage cannot be specified for some reaches and then calculated for others.

The Conductance value (C) may be calculated from the length of a reach (L) through a cell, the width of the stream channel (W) in the cell, the thickness of the streambed (M), and the vertical hydraulic conductivity of the streambed material (K) using the following formula.

$$C = \frac{K \times L \times W}{M}$$

Assigning Stream Segments

Due to the more complicated data requirements for the Streamflow-Routing Package, the **Stream** boundary condition in Visual MODFLOW is implemented using grid-independent line objects to represent each stream segment. These line objects are independent from the model grid and the attributes for each stream segment are linked to the individual line objects instead of being assigned to a specific model grid cell. As a result, the grid may be modified at any time without adversely affecting the stream data.

Stream boundary conditions can be assigned by selecting **Boundaries/Stream (STR)** from the **Input** section and using any of the left-hand toolbar options described below:

[Add Segment] Add a stream segment by digitizing a line along the stream **in the downstream direction**. Click the mouse pointer at the furthest upstream location of the segment and then digitize the line in the downstream direction along the length of the stream channel. Right-click at the location where the stream segment ends.

[Delete Segment] Delete one or more selected stream segments by clicking on the segments to delete.

[Move Segment] Move individual nodes of a stream segment, or move the entire stream segment, to a new location. Select a stream segment to highlight the nodes and then click-and-drag the node/segment to a new location.

[Edit Segment] Edit or assign the attributes for one or more stream segments.

The recommended process for assigning the **Stream** boundaries is to first assign the main stream channel(s) segment and then add the stream attributes for this channel. Then assign the tributaries and diversions as necessary and add the stream attributes for these segments. Keep in mind that each stream segment MUST be digitized in the downstream direction to ensure proper sequential numbering of the segments and the reaches within each segment. The data for each stream segment can be added immediately after each stream segment is added defined, or the data can be entered after the entire stream network has been added.

Adding a New Segment to an Existing Segment

- Click **[Add Segment]** from the left-hand toolbar
- Start digitizing the new segment by clicking the mouse pointer on the end node from an existing segment.
- A message will appear asking '**Snap to nearest node?**". Choose **[Yes]**.
- The new segment will be joined to the existing segment at this node location.
- Digitize a line along the new segment to the furthest downstream location
- Right-click the mouse pointer at the end point of the new segment.

Joining a Tributary Segment to an Existing Stream Segment

A tributary segment contributes flow to a main segment. A downstream segment can receive contributions from multiple tributary segments at the same location.

- Click **[Add Segment]** from the left-hand toolbar
- Digitize a line along the tributary segment, starting from the furthest upstream location, down to the point where it will join an existing segment.
- Right-click to end the tributary segment near a node from the existing segment.
- A message will appear asking '**Snap to nearest node?**". Choose **[Yes]**.
- The tributary segment will be joined to the existing segment at this node

location, and the existing segment will be split into two separate segments, an upstream segment and a downstream segment.
- If the existing segment already has data assigned to it, the end point values for the upstream segment and the start point values for the downstream segment will automatically be interpolated from the original data.

Adding Diversion Segments

A diversion segment is used to divert a specified flow from the main segment. Multiple diversions can be specified at the same location, but if the diverted flow is larger than the actual flow, the diverted flow will be set to zero.

- Click **[Add Segment]** from the left-hand toolbar
- Start digitizing the diversion segment by clicking the mouse pointer on a node from an existing segment where the streamflow will be diverted.
- A message will appear asking '**Snap to nearest node?**". Choose **[Yes]**.
- The diversion segment will be joined to the existing segment at this node location, and the existing segment will be split into two separate segments, an upstream segment and a downstream segment.
- If the existing segment already has data assigned to it, the end point values for the upstream segment and the start point values for the downstream segment will automatically be interpolated from the original data.
- Digitize a line along the diversion segment to the furthest downstream location
- Right-click the mouse pointer at the end point of the diversion segment.

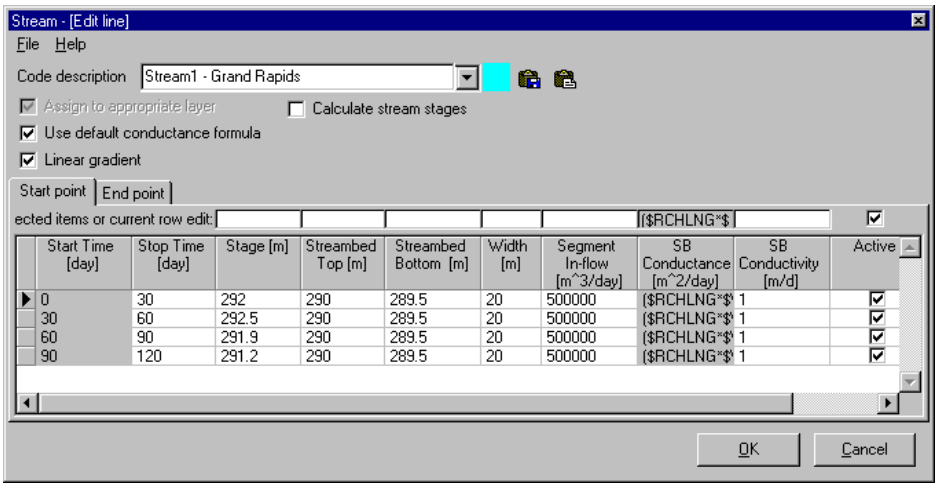
Adding a Node to a Segment

- Click **[Move Segment]** from the left-hand toolbar
- Click the segment to make it active
- Right-click on the new node location
- Select the **Add node** option

Entering Stream Data

Once the stream segments are added to the model, the Stream data for each stream segment must be assigned. To assign Stream data to one or more segments

- Click the **[Edit Segment]** button
- A **Select Segment** window will appear with a list of available stream segments (a green dot indicates the corresponding segment contains all of the required data, while a red dot indicates the corresponding segment still requires data).
- Choose the desired segment by clicking in the corresponding checkbox.
- Click the **[Edit]** button to open the **Stream** data input window shown below.



The **Code description** is described on page 104.

The **Assign to appropriate layer** option is described on page 104.

The U**se default conductance formula** option is described on page 105.

The **Linear gradient** option is described on page 105.

The **Calculate stream stages** option is used to indicate that the Stream Stage elevations will be calculated.

When a Stream boundary condition is assigned, the **Use default conductance formula** option is automatically selected.

If the **Use default conductance formula** option is selected, the Stream boundary condition requires the following data:

- **Stream Stage**: The free water surface elevation of the surface water body.
- **Streambed Top**: The elevation of the top of the seepage layer (bedding material) for the surface water body.
- **Streambed Top**: The elevation of the bottom of the seepage layer (bedding material) for the surface water body.
- **Width**: Width of the stream channel.
- **Segment Inflow**: Streamflow entering the first reach of the segment. Enter a value of -1 to indicate the Inflow is to be calculated using the outflow from the last reach of the upstream segment(s).
- **Streambed Conductance**: A numerical parameter representing the resistance to flow between the surface water body and the aquifer (this field is read-only and is calculated using the formula described below).
- **Streambed Kz**: Vertical hydraulic conductivity of the streambed material.

The default conductance formula is as follows:

$$\$COND = \frac{\$RCHLNG \text{ ¥ } \$WIDTH \text{ ¥ } \$K \text{ ¥ } \$UCTOCOND}{\$STOP - \$SBOT}$$

Where:

$COND	is the **Conductance**
$RCHLNG	is the reach length of the river line in each grid cell
$WIDTH	is the **River Width** in each grid cell
$K	is the **Riverbed Kz**
$UCTOCOND	is the conversion factor for converting the **$K** value to the same L and T units used by **$COND**
$STOP	is the **Streambed Top** elevation
$SBOT	is the **Streambed Bottom** elevation

If the **Use default conductance formula** option is turned off, the fields used for calculating the **Streambed Conductance** value (**Width** and **Streambed Kz**) are removed from the table and the **Streambed Conductance** field becomes a read/write field where any value or alternate formula may be entered.

If the **Calculate stream stage** option is selected, the Stream data input window will also prompt for the **Roughness** (Manning's roughness coefficient) of the stream channel. The **Slope** of the stream channel is not entered because it is automatically calculated using the change in the **Streambed Top** elevation from one grid cell to the next.

For details on entering boundary condition data refer to the section Entering Flow Boundary Condition Data on page 106.

For details on using mathematical formulas and array variable to define boundary condition data refer to the section Using Mathematical Formulas and Array Variables on page 108.

For details on importing transient boundary condition data refer to the section Importing Transient Boundary Condition Data on page 110.

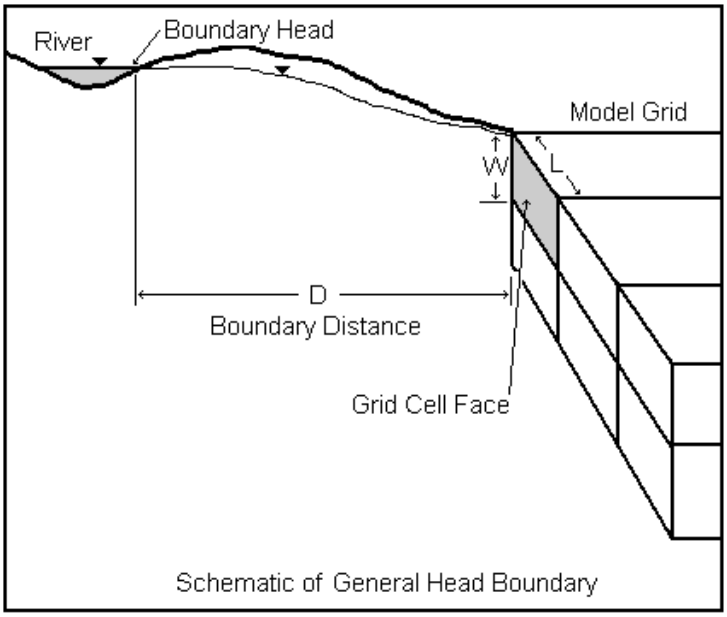
For details on erasing boundary conditions refer to the section Erasing Flow Boundary Conditions on page 116.

For details on copying boundary condition data refer to the section Copying Flow Boundary Conditions on page 116.

General-Head (GHB) Boundary Conditions

Visual MODFLOW supports the General-Head Boundary Package included with MODFLOW. The Visual MODFLOW input data for General-Head grid cells is stored in the *projectname*.VMB file (see Appendix A), while the MODFLOW input data for General-Head grid cells is stored in the *projectname*.GHB file (see MODFLOW-2000 Reference Manual .PDF file provided with the Visual MODFLOW installation CD-ROM).

The function of the General-Head Boundary (GHB) Package is mathematically similar to that of the River, Drain and ET Packages. Flow into or out of a cell from an external source is provided in proportion to the difference between the head in the cell and the reference head assigned to the external source. The purpose of this boundary condition is intended to be general, as indicated by its name, but the typical application of this boundary conditions is to represent heads in a model that are influenced by a large surface water body outside the model domain with a known water elevation. The purpose of using this boundary condition is to avoid unnecessarily extending the model domain outward to meet the element influencing the head in the model. As a result, the General Head boundary condition is usually assigned along the outside edges of the model domain. This scenario is illustrated in the following figure.



The primary differences between the General-Head boundary and the Constant Head boundary is:

- the model solves for the head value in the General-Head grid cells
- the General-Head grid cells do not act as infinite sources of water (i.e. General-

Head grid cells may become dry cells under some circumstances)

The General-Head Boundary Package requires the following information for each General-Head grid cell:

- **Boundary Head:** This is the head of the external source/sink. This head may be physically based, such as a large lake, or may be obtained through model calibration.
- **Conductance:** The conductance is a numerical parameter that represents the resistance to flow between the boundary head and the model domain.

In contrast to the River, Drain and ET Packages, the GHB Package provides no limiting value of head to bind the linear function in either direction. Therefore, as the head difference between a model cell and the boundary head increases, flow into or out of the cell continues to increase without limit. Accordingly, care must be used to ensure that unrealistic flows into or out of the system do not develop during the simulation.

The Conductance value may be physically based, representing the conductance associated with an aquifer between the model area and a large lake, or may be obtained through model calibration. The Conductance value (C) for the scenarios illustrated in the above figure may be calculated using the following formula:

$$C = \frac{(L \times W) \times K}{D}$$

Where,

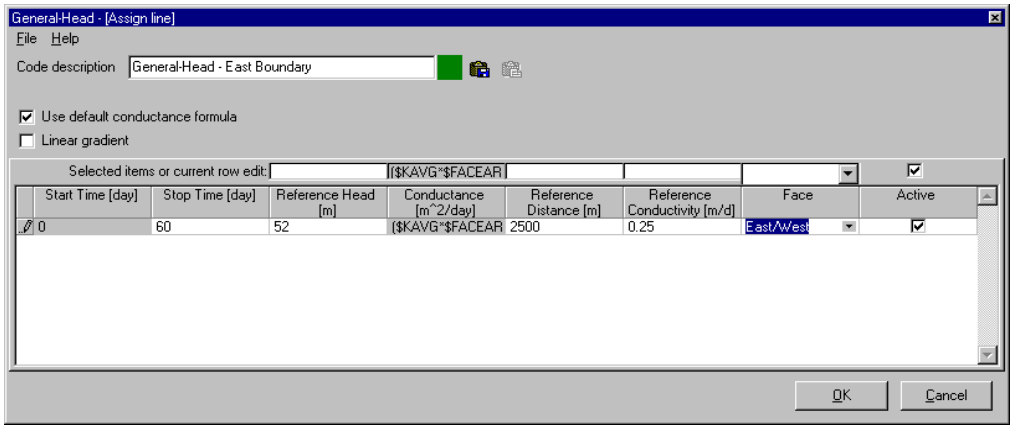
(L X W) is the surface area of the grid cell face exchanging flow with the external source/sink

K is the average hydraulic conductivity of the aquifer material separating the external source/sink from the model grid

D is the distance from the external source/sink to the model grid

General-Head boundary conditions can be assigned by selecting **Boundaries/General-Head (GHB)** from the **Input** section and using any of the **[Assign >]** options from the left-hand toolbar (described in the section Tools for Assigning and Editing Boundary Conditions on page 100).

Once the model grid cells are selected, a data input window will appear as shown in the following figure.



The **Code description** is described on page 104.

The U**se default conductance formula** option is described on page 105.

The **Linear gradient** option is described on page 105.

When a General-Head boundary condition is assigned, the **Use default conductance formula** option is automatically selected.

If the **Use default Conductance formula** option is selected, the General-Head boundary condition requires the following data:

- **Boundary Head:** The head value for the external source/sink
- **Conductance:** A numerical parameter representing the resistance to flow between the boundary head and the model domain (this field is read-only and is calculated using formula described below)
- **Boundary Distance:** The distance from the external source/sink to the General-Head grid cell
- **Average K:** The average hydraulic conductivity of the aquifer material separating the external source/sink from the model grid
- **Face:** The face of the grid cell exchanging flow with the external source/sink

The default formula used to calculate the Conductance value for the General-Head boundary is:

$$\$COND = \frac{\$KAVG \times \$FACEAREA \times \$UCTOCOND}{\$DIST}$$

Where:

$COND is the **Conductance** for each General-Head grid cell

$KAVG is the **Average K**

$FACEAREA is the surface area of the select grid cell **Face** for each General-Head grid cell

$UCTOCOND is the conversion factor for converting the **$K** value to the same L and T units used by **$COND**

$DIST is the **Boundary Distance**

If the **Use default conductance formula** option is not selected, the fields used for calculating the General-Head Conductance value (**Boundary Distance**, **Average K**, and **Face**) are removed from the table and the **Conductance** field becomes a read/write field where any value or alternate formula may be entered.

> **Note:** When Conductance values (or any other parameters) are calculated using a formula, the array variables and formulas are not saved together with the General-Head boundary data and cannot be recalled or modified at a later time. Visual MODFLOW only stores the **Boundary Head** and **Conductance** values for each grid cell.

For details on entering boundary condition data refer to the section Entering Flow Boundary Condition Data on page 106.

For details on using mathematical formulas and array variable to define boundary condition data refer to the section Using Mathematical Formulas and Array Variables on page 108.

For details on importing transient boundary condition data refer to the section Importing Transient Boundary Condition Data on page 110.

For details on editing boundary conditions data refer to the section Editing Flow Boundary Conditions on page 113.

For details on erasing boundary conditions refer to the section Erasing Flow Boundary Conditions on page 116.

For details on copying boundary condition data refer to the section Copying Flow Boundary Conditions on page 116.

Drain (DRN) Boundary Conditions

Visual MODFLOW supports the standard Drain Boundary Package included with MODFLOW. The Visual MODFLOW input data for Drain grid cells is stored in the *projectname*.VMB file (see Appendix A), while the MODFLOW input data for Drain grid cells is stored in the *projectname*.DRN file (see MODFLOW-2000 Reference Manual .PDF file provided with the Visual MODFLOW installation CD-ROM).

MODFLOW's Drain Package is designed to simulate the effects of features such as agricultural drains, which remove water from the aquifer at a rate proportional to the difference between the head in the aquifer and some fixed head or elevation. The Drain

package assumes the drain has no effect if the head in the aquifer falls below the fixed head of the drain.

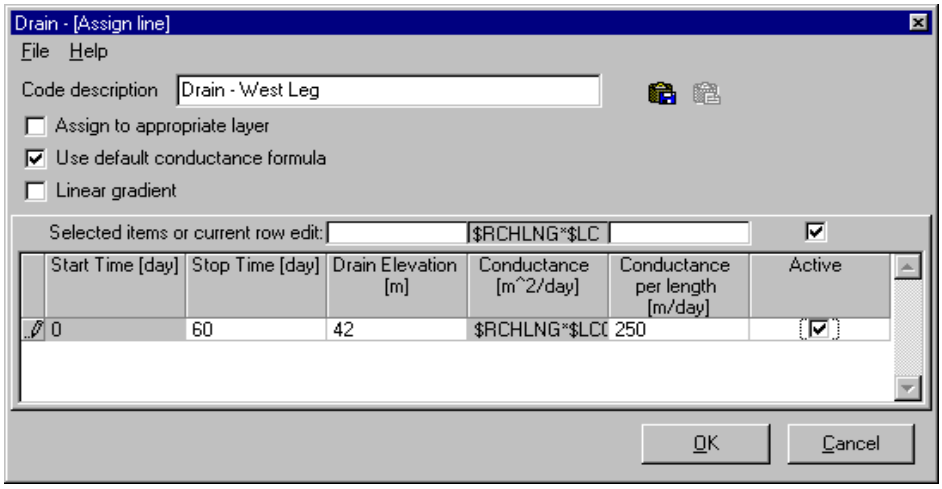
The Drain Package requires the following information as input for each cell containing this boundary condition:

- **Drain Elevation:** The drain elevation, or drain head of the free surface of water within the drain. The drain is assumed to run only partially full, so that the head within the drain is approximately equal to the median elevation of the drain.
- **Conductance:** The drain conductance is a lumped coefficient describing the head loss between the drain and the groundwater system. This loss is caused by converging flow patterns near the drain, the presence of foreign material around the drain, channel bed materials, the drain wall, and the degree to which the drain pipe openings may be blocked by chemical precipitates, plant roots, etc.

There is no general formulation for calculating drain conductance. In most situations, the detailed information required to calculate drain conductance is not available to the groundwater modeler. These details include the detailed head distribution around the drain, aquifer hydraulic conductivity near the drain, distribution of fill material, number and size of the drain pipe openings, the amount of clogging materials, and the hydraulic conductivity of clogging materials. It is common to calculate drain conductance from measured values of flow rate and head difference. Drain Conductance value is usually adjusted during model calibration.

Drain boundary conditions can be assigned by selecting **Boundaries/Drain (DRN)** from the **Input** section and using any of the **[Assign >]** options from the left-hand toolbar (described in the section Tools for Assigning and Editing Boundary Conditions on page 100).

Once the model grid cells are selected, a data input window will appear as shown in the following figure.



The **Code description** is described on page 104.

The **Assign to appropriate layer** option is described on page 104.

The U**se default conductance formula** option is described on page 105.

The **Linear gradient** option is described on page 105.

When a Drain boundary condition is assigned, the **Use default conductance formula** option is automatically selected.

If the **Use default Conductance formula** option is selected, the Drain boundary condition requires the following data:

- **Drain Elevation:** The head value for the external source/sink
- **Conductance:** A numerical parameter representing the resistance to flow between the boundary head and the model domain (this field is read-only and is calculated using formula described below)
- **Conductance per length/area:** The Conductance value per unit length/area of the Drain grid cells

If the grid cells were selected using the **[Assign >] Line** option, the default formula for the Drain Conductance is as follows:

$$\$COND = \$RCHLNG \times \$LCOND$$

If the grid cells were selected using **[Assign >] Single, [Assign >] Polygon**, or **[Assign >] Window**, the default conductance formula is as follows:

$$\$COND = \$DX \times \$DY \times \$SCOND$$

Where:

$COND	is the **Conductance**
$RCHLNG	is the reach length of the drain in each grid cell
$LCOND	is the **Conductance per unit length** of the drain in each grid cell
$SCOND	is the **Conductance per unit area** of the drain in each grid cell
$DX	is the length of each grid cell in the X-direction
$DY	is the length of each grid cell in the Y-direction

If the **Use default conductance formula** option is turned off, the fields used for calculating the Drain Conductance value (**Conductance per unit length/area**) are removed from the table and the **Conductance** field becomes a read/write field where any value or alternate formula may be entered.

Note: When Conductance values (or any other parameters) are calculated using a formula, the array variables and formulas are not saved together with the River boundary data and cannot be recalled or modified at a later time. Visual MODFLOW only stores the **Drain Elevation** and **Conductance** values for each grid cell.

For details on entering boundary condition data refer to the section Entering Flow Boundary Condition Data on page 106.

For details on using mathematical formulas and array variable to define boundary condition data refer to the section Using Mathematical Formulas and Array Variables on page 108.

For details on importing transient boundary condition data refer to the section Importing Transient Boundary Condition Data on page 110.

For details on editing boundary conditions data refer to the section Editing Flow Boundary Conditions on page 113.

For details on erasing boundary conditions refer to the section Erasing Flow Boundary Conditions on page 116.

For details on copying boundary condition data refer to the section Copying Flow Boundary Conditions on page 116.

Using Drains for a Seepage Face

In many cases, the Drain boundary condition is used to simulate a seepage face where groundwater discharges to the surface of the model. Typically, this situation is encountered along steep slopes or escarpments and the Drain boundary is assigned to the top layer of grid cells along the side of the slope such that the **Drain Elevation** corresponds to the ground surface elevation (or just slightly below ground surface). When the water level reaches the ground surface elevation it is removed by the drain boundary.

This type of scenario can be easily accommodated in Visual MODFLOW by using the **[Assign >] Polygon** option to select the grid cells along the seepage face, and then entering a **Drain Elevation** value of:

$BOT+$DZ-0.1

Where **$BOT** is the bottom elevation of each Drain grid cell and **$DZ** is the thickness of each Drain grid cell. This formula will assign a **Drain Elevation** value corresponding to 0.1 ft below the top elevation of each Drain grid cell.

Wall (HFB) Boundary Conditions

Visual MODFLOW supports the Horizontal Flow Barrier (HFB) Package included with MODFLOW. The Visual MODFLOW input data for HFB grid cells is stored in the *projectname*.VMB file (see Appendix A), while the MODFLOW input data for HFB

grid cells is stored in the *projectname*.HFB file (see MODFLOW-2000 Reference Manual .PDF file provided with the Visual MODFLOW installation CD-ROM).

The Horizontal-Flow-Barrier (HFB) Package, or Wall Boundary as it is referred to in Visual MODFLOW, was developed to simulate thin, vertical, low-permeability features that impede the horizontal flow of groundwater. This package allows such features to be simulated without the need to reduce grid spacing in an excessive number of model cells, thus enhancing model efficiency. These features are approximated as a series of horizontal flow barriers conceptually situated on the boundaries between adjacent cells in the finite difference grid.

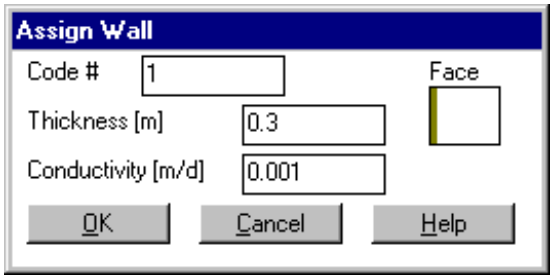
The key assumption underlying the HFB Package is the width of a barrier is negligibly small in comparison to the horizontal dimensions of the cells in the grid. Barrier width is not explicitly considered in the Package, but is represented in MODFLOW as a hydraulic characteristic defined as barrier hydraulic conductivity divided by barrier width.

The HFB Package requires the following information as input for each cell containing this boundary condition:

- **(I1, J1):** Row and column number of grid cell on one side of the barrier.
- **(I2, J2):** Row and column number of grid cell on the other side of the barrier.
- **Hydchr:** Hydraulic characteristic of the barrier (equivalent to hydraulic conductivity of the barrier divided by the width of the barrier).

Horizontal Flow Barriers (or Walls) can be assigned by selecting **Boundaries/Walls (HFB)** from the **Input** section and using either the **[Assign >] Single or [Assign >] Line** options from the left-hand toolbar (described in the section Tools for Assigning and Editing Boundary Conditions on page 100).

If the **[Assign >] Single** option is used, the following **Assign Wall** window will appear.



The parameters required for the Wall are as follows:

- **Code #**: A number used to identify different sections of a wall. This Code number may be used to copy the Wall to different layers of the model.
- **Thickness**: The width of the barrier wall.
- **Conductivity**: The hydraulic conductivity of the barrier wall.

- **Face**: Indicates the face of the grid cell against which the barrier wall is located. Click in the **Face** square to toggle the **Face** clockwise around the square.

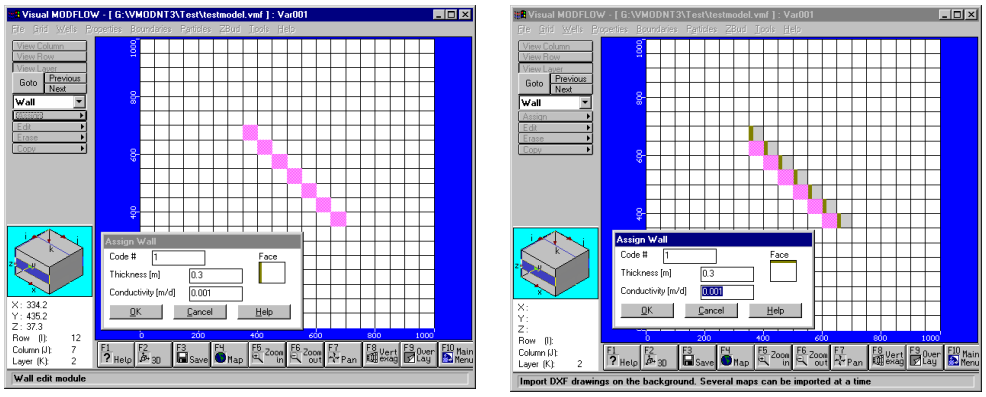
If the **[Assign >] Line** option is used, the **Assign Wall** window will prompt for **Thickness** and **Conductivity** values for the grid cell at both the **Start** point and **Stop** point of the line.

In Visual MODFLOW the Wall is assigned to only one face of each Wall grid cell. As a result, if the Barrier Wall is situated diagonal to the X or Y axis of the model grid, it must be assigned in two steps:

- **Step 1**: Select the grid cells located along the line of the wall and then select the appropriate **Face** of these grid cells where the wall will be assigned.
- **Step 2**: Select the grid cells adjacent to the first set and choose the face of the grid cell such that it will "seal" the openings in the Barrier Wall.

These two steps are demonstrated in the following figure.

Step 1 Step 2



Recharge (RCH) Boundary Conditions

Visual MODFLOW supports the Recharge Package included with MODFLOW. The Visual MODFLOW input data for Recharge is stored in the *projectname*.VMP file (see Appendix A), while the Recharge input data for MODFLOW is stored in the *projectname*.RCH file (see MODFLOW-2000 Reference Manual .PDF file provided with the Visual MODFLOW installation CD-ROM).

The Recharge Package is typically used to simulate aerial distributed recharge to the groundwater system. Most commonly, aerial recharge occurs as a result of precipitation that percolates into the groundwater system. However, the Recharge Package can potentially be used to simulate recharge from sources other than precipitation, for example, artificial recharge.

Note: The recharge rate is a parameter that is not often measured at a site, but rather it is assumed to be a percentage of the precipitation. This percentage typically ranges from 5% to 20% depending on many different factors including

- the predominant land use,
- the surface topography (slope), and
- the soil cover material

The U.S. EPA's HELP model is often used to estimate recharge rates for different zones within the model domain. Waterloo Hydrogeologic has developed a graphical interface for this program called Visual HELP that includes data from more than 3000 weather stations around the world. Contact a Waterloo Hydrogeologic representative for more information about Visual HELP and how it can be used to estimate recharge rates for groundwater modeling applications.

The Recharge Package requires a two-dimensional array of recharge values for each grid cell in the horizontal plane, and an optional two-dimensional array of the layer numbers where the recharge will be applied for grid cell in the horizontal plane.

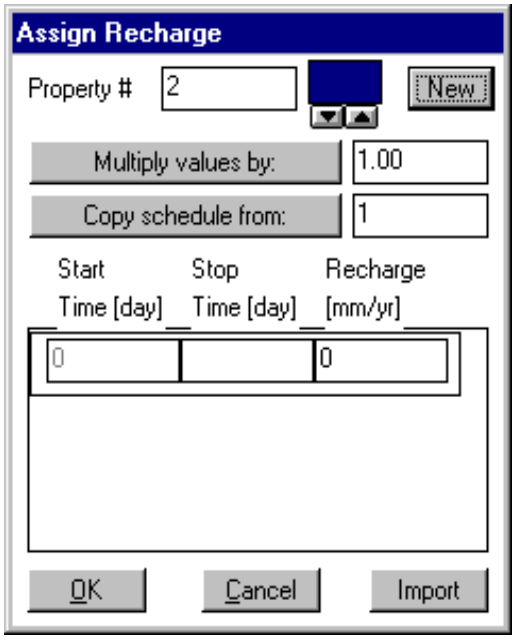
Since natural recharge enters the groundwater system at the ground surface, Visual MODFLOW only allows recharge values to be assigned to Layer 1 while in View Layer mode. This allows all recharge zones to be visible at the same time in the same layer. By default, Visual MODFLOW will set the recharge to be applied to the upper-most active (wet) layer of the model for each vertical column of grid cell. However, this setting may be modified in the **Run** section under the **MODFLOW/Recharge** menu (see section Recharge Settings on page 174).

Assigning Recharge Zones

The Recharge boundary condition can be assigned by selecting **Boundaries/Recharge (RCH)** from the **Input** section. Upon entering the **Recharge** screen for the first time, a pop-up window will require a default time schedule of Recharge values. This default time schedule is used to initially populate the two-dimensional array of Recharge values. Once the default values are entered, spatially variable Recharge zones may be assigned throughout Layer 1.

Recharge zones can be assigned using the **[Assign >]** options from the left-hand toolbar (described in the section Tools for Assigning and Editing Boundary Conditions on page 100). The Recharge boundary conditions are assigned to the model using different colored zones to represent different Recharge values. Visual MODFLOW supports an unlimited number of Recharge zones.

Once the model grid cells are selected for a Recharge zone, an **Assign Recharge** window will appear as shown in the following figure and described below.



The **Property #** field identifies the Recharge zone being assigned. Each different zone is represented by a different color indicated in the box beside the **Property #** field. The color of each zone is automatically linked to the zone number and cannot be customized.

The Recharge values for each zone can be viewed by using the up and down arrows to scroll through the existing zones, or by entering the integer number of the desired zone in the **Property #** field.

The **[Multiply values by:]** button is used to multiple all values for the selected Recharge zone by the specified multiplication factor. This multiplication factor will be applied to the original Recharge values present prior to pressing the button (i.e. a factor of "1" will return the original values).

The **[Copy schedule from:]** button is used to copy the Recharge time schedule from an existing zone to the current zone. Once the Recharge time schedule is copied, the **[Multiply values by:]** button may be used to modify the values.

Creating a New Recharge Zone

To create a new Recharge zone:

- Use the **[Assign >]** options in the Recharge screen to select the desired grid cells where the zone will be located.
- When the **Assign Recharge** window appears, press the **[New]** button.
- The Property # automatically increments and a new Recharge zone is created with an empty time schedule.
- Enter the **Stop Time** and **Recharge** values for the first time period.
- Press the **<Enter>** key to create a new time period, or click the **[OK]** button to accept this value (see instructions below for importing transient recharge data).

Note: If transient Recharge data is entered, the Recharge value for the first time period will be used for steady-state simulations.

The **[Copy schedule from:]** button can be used to copy the Recharge time schedule from an existing zone to the current zone. Once the Recharge time schedule is copied, the **[Multiply values by:]** button may be used to modify the Recharge values.

Editing Recharge Values

To modify the data for an existing Recharge Zone, select **[Edit >] Property** from the left-hand toolbar and an **Edit Recharge** window will appear. The **Edit Recharge** window has the same appearance and functionality as the **Assign Recharge** window described above.

The Recharge values for each zone can be viewed by using the up and down arrows to scroll through the existing zones, or by entering the integer number of the desired Recharge zone in the **Property #** field.

The **[Multiply values by:]** button is used to multiple all values for the selected Recharge zone by the specified multiplication factor. This multiplication factor will be applied to the original Recharge values present prior to pressing the button (i.e. a factor of "1" will return the original values).

Importing Transient Recharge Values

Transient recharge data can be imported for a selected Recharge zone using the **[Import]** button in the **Assign/Edit Recharge** window.

The imported file must be a space delimited file containing three columns of data with no header information. The three columns of space delimited data must contain:

Start Time Stop Time Recharge

The **Stop Time** for each time period must always coincide with the **Start Time** for the next time period. In addition, the units of the imported data must match those set during the model's creation.

Visual HELP v.2.2 allows for the calculation and export of recharge schedules. The files created are in the format required by Visual MODFLOW and simply need to be imported as described above. Again, caution must be taken to ensure that the units of the imported file match those used in the Visual MODFLOW model.

Deleting Recharge Zones

Once Recharge values are assigned to the model, each grid cell in Layer 1 will always require a Recharge value. As a result, Recharge zones may not be deleted, but rather replaced by a different zone. Use the **[Assign >]** options to assign a different Recharge zone in place of the unwanted zone.

Evapotranspiration (EVT) Boundary Conditions

Visual MODFLOW supports the Evapotranspiration Package included with MODFLOW. The Visual MODFLOW input data for Evapotranspiration is stored in the *projectname*.VMP file (see Appendix A), while the Evapotranspiration input data for MODFLOW is stored in the *projectname*.EVT file (see MODFLOW-2000 Reference Manual .PDF file provided with the Visual MODFLOW installation CD-ROM).

The Evapotranspiration Package simulates the effects of plant transpiration, direct evaporation and seepage at the ground surface by removing water from the saturated groundwater regime.

The Evapotranspiration Package requires the following information:

- **Evapotranspiration rate:** The rate of evapotranspiration as it occurs when the water table elevation is equal to the top of the grid cell elevation
- **Extinction Depth:** The depth below the top of grid cell elevation where the evapotranspiration rate is negligible.

The Evapotranspiration Package approach is based on the following assumptions:

- When the water table is at or above the ground surface (top of layer 1), evapotranspiration loss from the water table occurs at the maximum rate specified by the user.
- When the elevation of the water table is beneath the surface elevation less the 'extinction depth', or is beneath layer 1, evapotranspiration from the water table is negligible.
- Between these limits, evapotranspiration from the water table varies linearly with water table elevation.

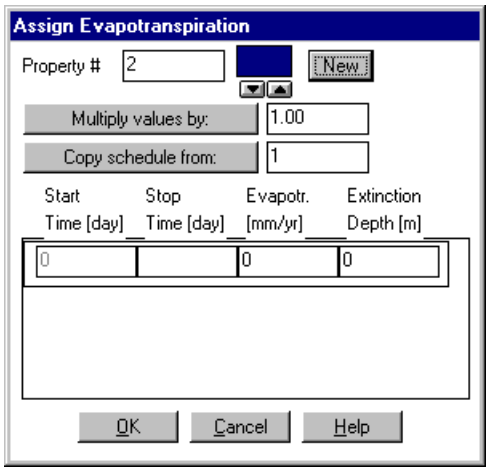
Since evapotranspiration from the groundwater system usually occurs at or near the ground surface, Visual MODFLOW only allows Evapotranspiration values to be assigned to Layer 1 while in View Layer mode. This allows all Evapotranspiration zones to be visible at the same time in the same layer.

Assigning Evapotranspiration Zones

The Evapotranspiration boundary condition can be assigned by selecting **Boundaries/ Evapotranspiration (EVT)** from the **Input** section. Upon entering the **Evapotranspiration** screen for the first time, a pop-up window will require a default time schedule of Evapotranspiration values. This default time schedule is used to initially populate the two-dimensional array of Evapotranspiration values. Once the default values are entered, spatially variable Evapotranspiration values may be entered by defining different Evapotranspiration zones in Layer 1.

Evapotranspiration zones can be assigned using the **[Assign >]** options from the left-hand toolbar (described in the section Tools for Assigning and Editing Boundary Conditions on page 100). Each Evapotranspiration zone represents a different set of Evapotranspiration values. Visual MODFLOW supports an unlimited number of Evapotranspiration zones.

Once the model grid cells are selected for an Evapotranspiration zone, an **Assign Evapotranspiration** window will appear as shown in the following figure and described below.



The **Property #** field identifies the Evapotranspiration zone being assigned. Each zone is represented by a different color indicated in the box beside the **Property #** field. The color of each zone is automatically linked to the zone number and cannot be customized.

The Evapotranspiration values for each zone can be viewed by using the up and down arrows to scroll through the existing zones, or by entering the integer number of the desired zone in the **Property #** field.

The **[Multiply values by:]** button is used to multiple all values for the selected Evapotranspiration zone by the specified multiplication factor. This multiplication factor will be applied to the original Evapotranspiration values present prior to pressing the button (i.e. a factor of “1” will return the original values).

The **[Copy schedule from:]** button is used to copy the Evapotranspiration time schedule from an existing zone to the current zone. Once the Evapotranspiration time schedule is copied, the **[Multiply values by:]** button may be used to modify the Evapotranspiration values.

Creating a New Evapotranspiration Zone

To create a new Evapotranspiration zone:

- Use the **[Assign >]** options in the Evapotranspiration screen to select the desired grid cells where the zone will be located.
- When the **Assign Evapotranspiration** window appears, press the **[New]** button.
- The Property # automatically increments and a new zone is created with an empty Evapotranspiration time schedule.
- Enter the **Stop Time** and **Evapotranspiration** values for the first time period.
- Press the **<Enter>** key to create a new time period, or click the **[OK]** button to accept this value.

Note: If transient Evapotranspiration data is entered, the Evapotranspiration value for the first time period will be used for steady-state simulations.

The **[Copy schedule from:]** button can be used to copy the Evapotranspiration time schedule from an existing zone to the current zone. Once the Evapotranspiration time

schedule is copied, the **[Multiply values by:]** button may be used to modify the Evapotranspiration values.

Editing Evapotranspiration Values

To modify the data for an existing Evapotranspiration Zone, select **[Edit >] Property** from the left-hand toolbar and an **Edit Evapotranspiration** window will appear. The **Edit Evapotranspiration** window has the same appearance and functionality as the **Assign Evapotranspiration** window described above.

The Evapotranspiration values for each Evapotranspiration zone can be viewed by using the up and down arrows to scroll through the existing zones, or by entering the integer number of the desired zone in the **Property #** field.

The **[Multiply values by:]** button is used to multiple all values for the selected Evapotranspiration zone by the specified multiplication factor. This multiplication factor will be applied to the original Evapotranspiration values present prior to pressing the button (i.e. a factor of “1” will return the original values).

Deleting Evapotranspiration Zones

Once Evapotranspiration values are assigned to the model, each grid cell in Layer 1 will always require a Evapotranspiration value. As a result, Evapotranspiration zones may not be deleted, but rather replaced by a different zone. Use the **[Assign >]** options to assign a different Evapotranspiration zone in place of the unwanted zone.

3.5.3 Mass Transport Boundary Conditions

The solution of the governing equation for mass transport requires the specification of boundary conditions. For the mass transport model supported by Visual MODFLOW there are four options for specifying transport boundary conditions:

- **Constant Concentration**
- **Recharge Concentration**
- **Evapotranspiration Concentration**
- **Point Source**

The following sections provide a description of the data requirements for each of these boundary condition types, and the options for assigning, editing and importing the required data.

Constant Concentration Boundary Conditions

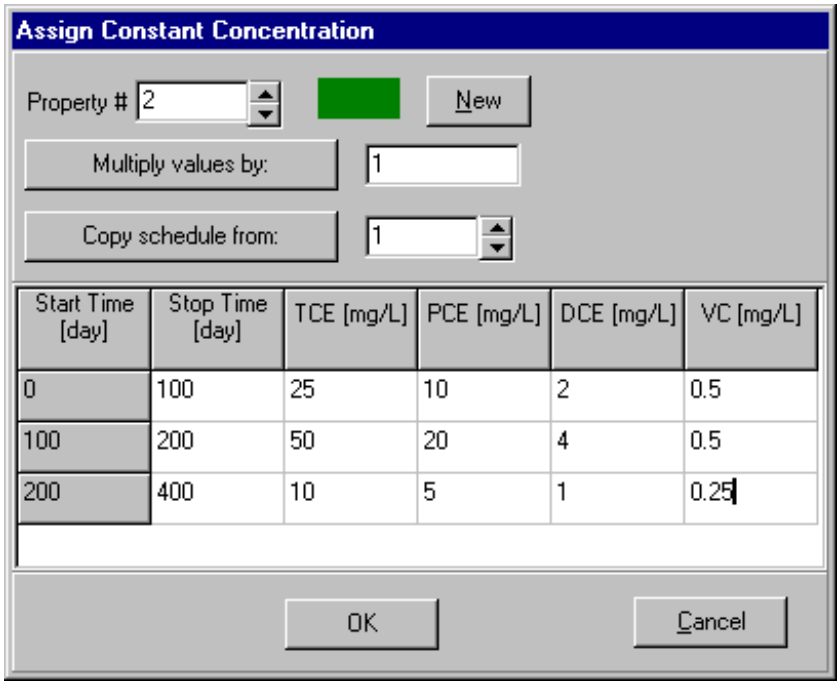
The Visual MODFLOW input data for Constant Concentration boundary conditions is stored in the *projectname*.MTN file (see Appendix A), while the Constant Concentration input data for MT3Dxx/RT3D is stored in the *projectname*.SSM file (see

MT3Dxx/RT3D Reference Manual .PDF file provided on the Visual MODFLOW installation CD-ROM).

The Constant Concentration boundary condition acts as a contaminant source providing solute mass to the model domain in the form of a known concentration in a grid cell. An example of such a boundary condition is a spill that provides dissolved phase contamination at a fixed concentration for a relatively long period of time. In some cases, the Constant Concentration boundary condition may also act as a sink by taking mass out of the domain.

Assigning Constant Concentration Zones

Constant Concentration boundary conditions can be assigned by selecting **Boundaries/ Constant Concentration** from the top menu bar and using the **[Assign >]** options from the left-hand toolbar (described in the section Tools for Assigning and Editing Boundary Conditions on page 100). Once the model grid cells are selected, the **Assign Constant Concentration** window will appear as shown below.



Constant Concentration boundary conditions are assigned using different colored zones to represent different sets of concentration values for each Species. Each zone requires specified concentration values for each Species at each time period. Typically, different zones will be used for different release locations within the same model.

The **Property #** field identifies the Constant Concentration zone being assigned. Each zone is represented by a different color indicated in the box beside the **Property #** field.

The color of each zone is automatically linked to the zone number and cannot be customized.

The Constant Concentration values for each zone can be viewed by using the up and down arrows to scroll through the existing zones, or by entering the integer number of the desired Constant Concentration zone in the **Property #** field.

The **[Multiply values by:]** button is used to multiple all values for the selected Constant Concentration zone by the specified multiplication factor. This multiplication factor will be applied to the original Constant Concentration values present prior to pressing the button (i.e. a factor of "1" will return the original values).

The **[Copy schedule from:]** button is used to copy the Constant Concentration time schedule from an existing Constant Concentration zone to the current Constant Concentration zone. Once the Constant Concentration time schedule is copied, the **[Multiply values by:]** button may be used to modify the values.

Creating a New Constant Concentration Zone

To create a new Constant Concentration zone:

- Use the **[Assign >]** options in the Constant Concentration screen to select the desired grid cells where the zone will be located.
- When the **Assign Constant Concentration** window appears, press the **[New]** button.
- The Property # automatically increments and a new Constant Concentration zone is created with an empty time schedule.
- Enter the **Stop Time** and **Concentration** values for the first time period.
- Press the **<Enter>** key to create a new time period, or click the **[OK]** button to accept this value.

Note: If the simulation time is longer than the time specified for the Constant Concentrations, then Visual MODFLOW assumes the concentration source has been removed from the system.

The **[Copy schedule from:]** button can be used to copy the Constant Concentration time schedule from an existing zone to the current zone. Once the Constant Concentration time schedule is copied, the **[Multiply values by:]** button may be used to modify the values.

Editing Constant Concentration Values

To modify the data for an existing Constant Concentration zone, select **[Edit >] Property** from the left-hand toolbar and an **Edit Constant Concentration** window will appear. This window has the same appearance and functionality as the **Assign Constant Concentration** window described above.

The concentration data for each Constant Concentration zone can be viewed by using the up and down arrows to scroll through the existing zones, or by entering the integer number of the desired zone in the **Property #** field.

The **[Multiply values by:]** button is used to multiple all values for the selected Constant Concentration zone by the specified multiplication factor. This multiplication factor will be applied to the original Constant Concentration values present prior to pressing the button (i.e. a factor of "1" will return the original values).

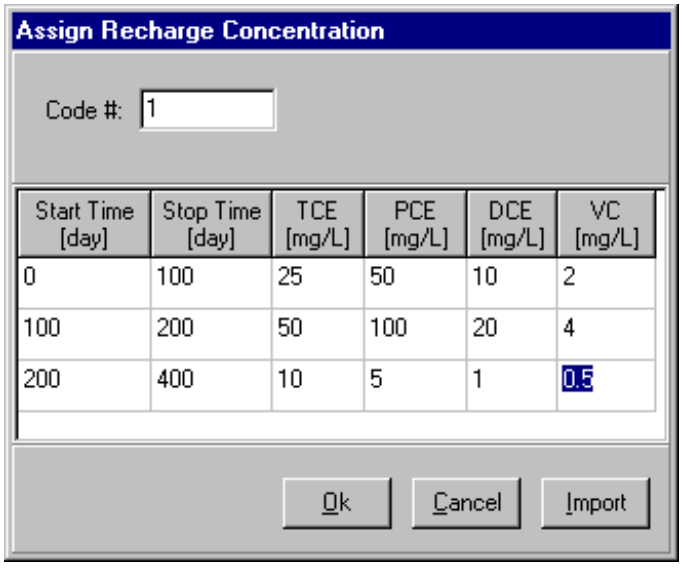
Recharge Concentration Boundary Conditions

The Visual MODFLOW input data for Recharge Concentration boundary conditions is stored in the *projectname*.MTH file (see Appendix A), while the Recharge Concentration input data for MT3Dxx/RT3D is stored in the *projectname*.SSM file (see MT3Dxx/RT3D Reference Manual .PDF file provided on the Visual MODFLOW installation CD-ROM).

The Recharge Concentration boundary condition specifies the concentration of each Species accompanying the Recharge flux specified in the flow model.

Assigning Recharge Concentrations

Recharge Concentration boundary conditions can be assigned by selecting **Boundaries/Recharge Concentration** from the top menu bar and using the **[Assign >]** options from the left-hand toolbar (described in the section Tools for Assigning and Editing Boundary Conditions on page 100). Once the model grid cells are selected the **Assign Recharge Concentration** window will appear as shown below.



Recharge Concentration grid cells are identified with a pink colored grid cell. Each set of Recharge Concentration grid cells may be assigned a different **Code #** to be used for identification and for copying the Recharge Concentration grid cells to a different layer.

Each Code # requires concentrations to be specified for each Species at each time period.

Importing Transient Recharge Concentration Data

Transient Recharge Concentration data can be imported for a selected Recharge Concentration **Code #** using the **[Import]** button in the **Assign/Edit Recharge Concentration** window.

The imported file must be a space delimited file containing three (or more) columns of data with no header information. The three (or more) columns of space delimited data must contain:

Start Time Stop Time RConc1 RConc2 RConc3..... RConcN

Where **RConcN** is the Recharge Concentration for the Nth Species being simulated by the model. The **Stop Time** for each time period must always coincide with the **Start Time** for the next time period, and a concentration value must be available for each Species in the model. In addition, the units of the imported data must match those set during the model's creation.

WHI Unsat Suite v.2.2 allows for the calculation and export of recharge concentration schedules. The files created are in the format required by Visual MODFLOW and simply need to be imported as described above. Again, caution must be taken to ensure that the units of the imported file match those used in the Visual MODFLOW model.

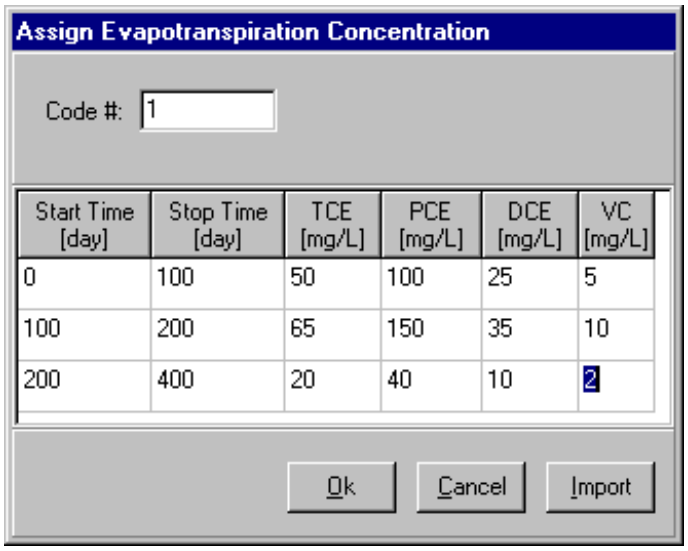
Evapotranspiration Concentration Boundary Conditions

The Visual MODFLOW input data for Evapotranspiration Concentration boundary conditions is stored in the *projectname*.MTV file (see Appendix A), while the Evapotranspiration Concentration input data for MT3Dxx/RT3D is stored in the *projectname*.SSM file (see MT3Dxx/RT3D Reference Manual .PDF file provided on the Visual MODFLOW installation CD-ROM).

The Evapotranspiration Concentration boundary condition specifies the concentration of each Species accompanying the Evapotranspiration flux specified in the corresponding flow model.

Assigning Evapotranspiration Concentrations

Evapotranspiration Concentration boundary conditions can be assigned by selecting **Boundaries/Evapotr. Concentration** from the top menu bar and using the **[Assign >]** options from the left-hand toolbar (described in the section Tools for Assigning and Editing Boundary Conditions on page 100). Once the model grid cells are selected the **Assign Evapotranspiration Concentration** window will appear as shown below.



Evapotranspiration Concentration grid cells are identified with a dark-green colored grid cell. Each set of Evapotranspiration Concentration grid cells may be assigned a different **Code #** to be used for identification and for copying the Evapotranspiration Concentrations grid cells to a different layer.

Each Code # requires concentrations to be specified for each Species at each time period.

Importing Transient Evapotranspiration Concentration Data

Transient Evapotranspiration Concentration data can be imported for a selected Evapotranspiration Concentration **Code #** using the **[Import]** button in the **Assign/Edit Evapotranspiration Concentration** window.

The imported file must be a space delimited file containing three (or more) columns of data with no header information. The three (or more) columns of space delimited data must contain:

Start Time Stop Time EConc1 EConc2 EConc3..... EConcN

Where **EConcN** is the Evapotranspiration Concentration for the Nth Species being simulated by the model.The **Stop Time** for each time period must always coincide with the **Start Time** for the next time period, and a concentration value must be available for each Species in the model. In addition, the units of the imported data must match those set during the model's creation.

WHI Unsat Suite v.2.2 allows for the calculation and export of Evapotranspiration concentration schedules. The files created are in the format required by Visual MODFLOW and simply need to be imported as described above. Again, caution must

be taken to ensure that the units of the imported file match those used in the Visual MODFLOW model.

Point Source Boundary Conditions

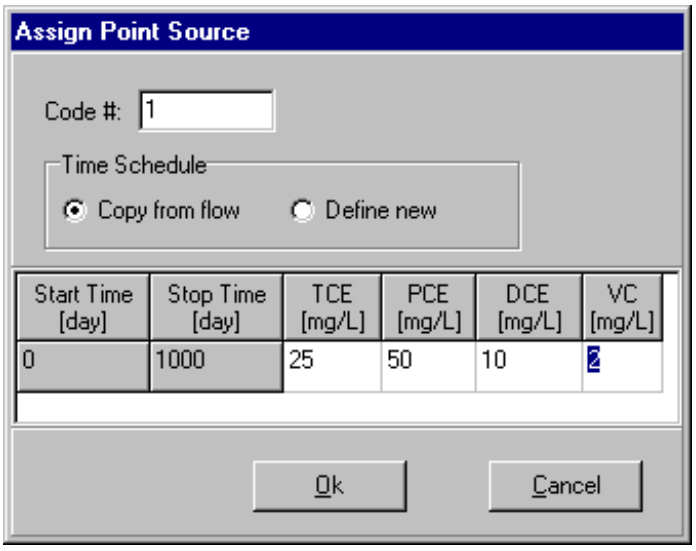
The Visual MODFLOW input data for Point Source boundary conditions is stored in the *projectname*.MTS file (see Appendix A), while the Evapotranspiration Concentration input data for MT3Dxx/RT3D is stored in the *projectname*.SSM file (see MT3Dxx/RT3D Reference Manual .PDF file provided on the Visual MODFLOW installation CD-ROM).

The Point Source boundary condition specifies the concentration of each Species entering or leaving the model through a flow boundary condition grid cell specified in the corresponding flow model.

Assigning Point Sources

Point Source boundary conditions can be assigned by selecting **Boundaries/Point Source** from the top menu bar and using the **[Assign >]** options from the left-hand toolbar (described in the section Tools for Assigning and Editing Boundary Conditions on page 100).

The Point Source boundary condition may ONLY be assigned in grid cells containing a flow boundary condition. Once the model grid cells are selected the **Assign Point Source** window will appear as shown below.



Point Source grid cells are identified with a yellow colored grid cell. Each set of Point Source grid cells may be assigned a different **Code #** to be used for identification.

The **Time Schedule** frame has two options for defining the time schedule for the Point Source:

- **Copy from flow** copies the time schedule from the existing flow boundary conditions
- **Define new** allows for a new time schedule to be entered

Each **Code #** requires concentrations to be specified for each Species at each time period.

> **Note:** If a flow boundary condition is deleted from the flow model, the Point Source boundary condition corresponding to this grid cell will also be deleted from the model.

3.6 Particles (MODPATH)

The computer program MODPATH was developed by the USGS (Pollock, 1989) to calculate three-dimensional particle tracking from steady-state flow simulations output obtained using MODFLOW. MODPATH can be used to compute three-dimensional pathlines and the position of particles at specified points in time.

MODPATH uses a semi-analytical particle-tracking scheme. The method is based on the assumption that each directional velocity component varies linearly within a grid cell in its own co-ordinate direction. This assumption allows an analytical expression to be obtained describing the flow path within a grid cell. Given the initial position of a particle anywhere in a cell, the co-ordinates of any other point along its path line within the cell, and the time of travel between them, can be computed.

Documentation of the theoretical and numerical implementation of MODPATH are given in the USGS Open File Report 89-381, "Documentation of Computer Programs to Compute and Display Pathlines Using Results from the U.S. Geological Survey Modular Three-Dimensional Finite-Difference Ground-Water Model, by David W. Pollock." which is included in the MODFLOW Packages Reference Manual.

To access the MODPATH input screen, click on **[Particles]** at the top of the Input section and the following additional menu items will appear on the side menu bar.

[Add]	Add a **Single** particle, a **Line** of particles, or a **Circle** of particles.
[Delete]	Deletes selected particles or groups of particles.
[Tracking]	Changes the particle tracking direction of selected particles or groups of particles.
[Copy]	Copy particles to other layers, columns or rows.
[Release Time]	Specify the release time for forward particles (for use with the transient version of MODPATH).

Any particles input will be visible in both cross-section and plan view.

Adding Single Particles

- Click on **[Add >] Add Particle** on the left-hand toolbar.
- A **Single Particle** window will appear.
- Select the tracking direction for the particles and then click on the desired particle locations in the model grid.
- Click **[OK]** when all particle locations have been assigned.

Adding a Line of Particles

- Click on **[Add >] Add Line** on the left-hand toolbar.
- Move the mouse pointer to the starting point of the line.
- Left-click to anchor the starting location of the line, and then left-click again on the end point of the line.
- A **Line Particle** window will appear.
- Select the particle tracking direction and the number of particles along the line.
- Click **[OK]** to assign the line of particles.

If a line of particles is assigned across a variable surface, the particles will all be assigned at an elevation equal to the mid-point of the grid cell at the starting point of the line.

Adding a Circle of Particles

A circle of backward tracking particles are generally assigned around a pumping well in order to determine the capture zone for that well.

- Click on **[Add >] Add Circle** on the left-hand toolbar.
- Move the mouse pointer to the centre of the circle.
- Left-click to anchor the centre location of the circle, and then left-click again at the desired radius of the circle.
- A **Circle Particle** window will appear.
- Select the particle tracking direction and the number of particles around the circle.
- Click **[OK]** to assign the circle of particles.

Deleting Particles

- Click the **[Delete] button** on the left-hand toolbar.
- A **Delete Particle** window will appear.
- Use the mouse pointer to select the particles or groups of particles to delete
- Click **[OK]** to delete the selected particles.

Changing the Particle Tracking Direction

Once particle are assigned to the model the tracking direction may be changed at any time without re-assigning the particles.

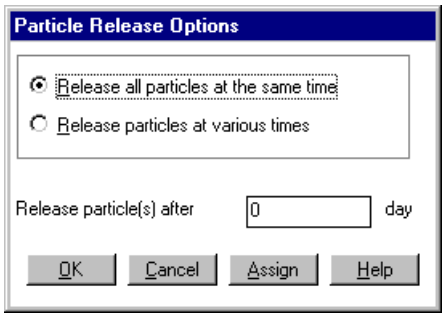
- Click the **[Tracking]** button on the left-hand toolbar.
- Use the mouse pointer to set the tracking direction of selected particles or groups of particles. Left-click to set to forward tracking (green color particles), or right-click to set to backward tracking (red color particles).

Copying Particles

- Click the **[Copy]** button on the left-hand toolbar.
- A **Copy Particle** window will appear.
- Use the mouse pointer to select the particles or group of particles to copy to another layer.
- Highlight the target layer(s) where the particles will be copied to (the **[Select All]** button selects all layers).
- Click **[OK]** to copy the selected particles to the selected layers.

Particle Release Time

The particle release time is the time when the particle is released from the location where it is assigned and allowed to travel with the groundwater flow. This option is only appropriate for transient flow models where the groundwater flow directions are changing with time.



The particle release times for forward tracking particles can be specified by pressing the **[Release Time]** option on the left-hand toolbar. The following **Particle Release Options** window appears with two options for specifying particle release times.

- **Release all particles at the same time** will assign the same release time to all forward tracking particles in the model.
- **Release particles at various times** will set the release time for selected particles or groups of particles.

Reference times for backward tracking particles may be assigned in the **Run** section by selecting **MODPATH/Reference Times** from the top menu bar (see section Reference Time Settings on page 184).

Particle Discharge Options

The particle discharge options for MODPATH are available in the **Run** section of Visual MODFLOW under the **MODFPATH/Discharge Options** in the top menu bar. These options are explained in the section Discharge Options on page 182.

3.7 Zone Budget

Zone Budget calculates sub-regional water budgets using results from steady-state or transient MODFLOW simulations. Zone Budget calculates budgets by tabulating the budget data that MODFLOW produces using the cell-by-cell flow option. The user simply specifies the sub-regions for which budgets will be calculated. These sub-regions are entered as 'zones' analogous to the way that properties, such as hydraulic conductivity, are entered. Following a simulation, Zone Budget results can be read in the **Output** section under the **Graphs** item in the top menu bar.

The theoretical and numerical implementation of Zone Budget is described in the USGS Report "A Computer Program for Calculating Subregional Water Budgets Using Results from the U.S. Geological Survey Modular Three-Dimensional Finite-Difference Groundwater Flow Model, by Arlen W. Harbaugh", which is included in the MODFLOW Packages Reference Manual.

After selecting **[Zbud]** from the top menu bar the following additional side menu items appear:

[Assign >] Assign user-defined water budget zones to **Single** grid cells, by digitizing a **Polygon** around a group of grid cells, or by stretching a rectangular **Window** around a group of grid cells.

[Copy >] Copy selected water budget zones from one layer to another layer.

[Database] Display a list of all defined water budget zones, with colors corresponding to the zone number.

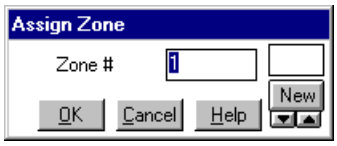
[Observations] Enter flow observations for selected zones in the model.

Assigning Zones

Zone Budget Zones can be assigned by selecting **Zbud** from the top menu bar of the **Input** section and using any of the **[Assign >]** options described below:

- **[Assign >] Single** is used to select individual grid cells where the zone will be assigned. Hold the mouse button down to select multiple grid cells, or click the right mouse button to unselect grid cells.
- **[Assign >] Polygon** is used to digitize a polygon around the group of grid cells where the zone will be assigned. Left-click at the start point of the polygon to begin digitizing the shape of the polygon and right-click near the start point to close the polygon.
- **[Assign >] Window** is used to stretch a Window (rectangle) around the group of grid cells where the zone will be assigned. Left-click at one corner of the window and left-click again at the opposite corner to define the window dimensions.

Once the Zone Budget grid cells are selected, the **Assign Zone** window will appear as shown in the following figure.

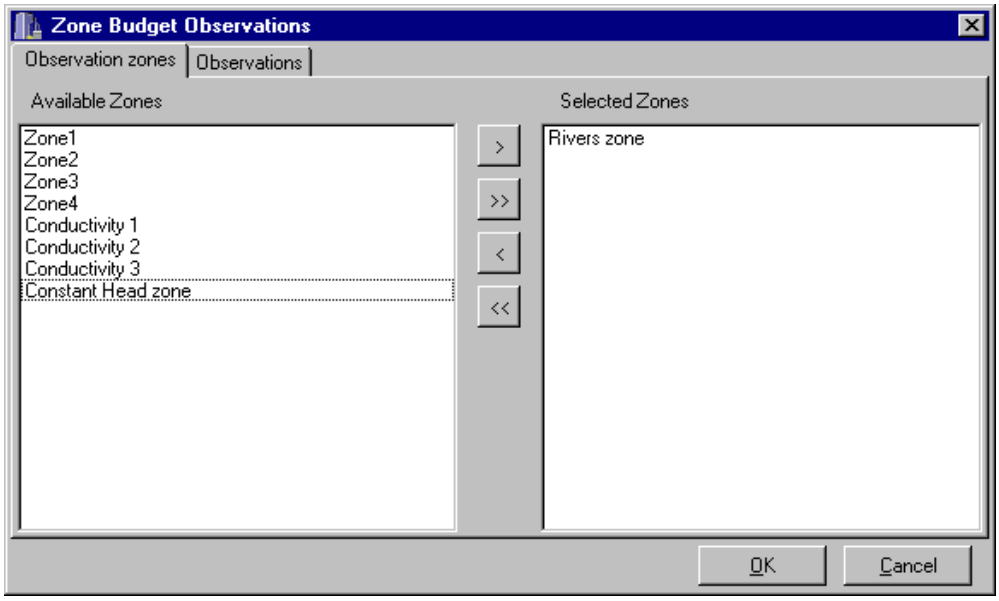


Each Zone Budget Zone is defined by a Zone # and is identified by a representative color. Click the **[New]** button to assign a new Zone Budget Zone to the selected grid cells, or use the up and down arrow buttons to step through the available zones.

Flow Observations

Flow observations, such as baseflow to a stream, or flux across a boundary, are very useful for calibrating a groundwater flow model against data other than just head measurements. The utilization of flow observations provides a stronger line of evidence to verify the model predictions and is particularly useful in models where the water table is relatively flat.

Flow observations may be entered by selecting the **[Observations]** button from the left-hand toolbar of the **Zbud** screen. The following **Zone Budget Observations** window will appear.

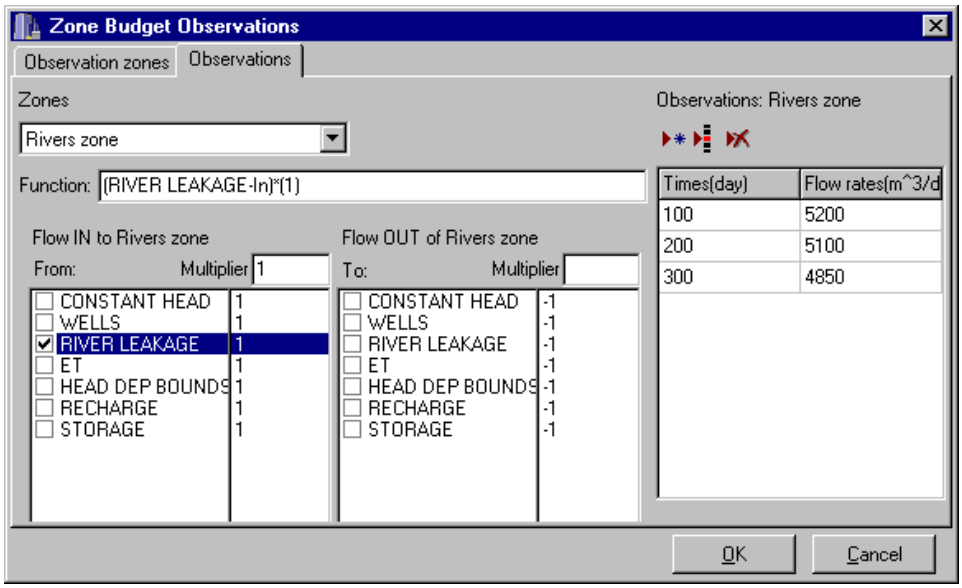


The **Observation Zones** tab lists the **Available Zones** in the model, and the **Selected Zones** where flow observations will be defined. By default, Visual MODFLOW will include zones for each flow boundary condition and each Conductivity zone.

Use the arrow buttons to move selected zones from the **Available Zones** list to the **Selected Zones** list, or vice versa.

Note: If any of the Conductivity zones or flow boundary conditions are used in a flow observation and then are later deleted from the model, Visual MODFLOW will NOT automatically update the associated flow observations. As a result some problems may occur if WinPEST is being used to calibration the model using these 'corrupted' flow observations.

The **Observations** tab (see figure below) is where the flow observations may be entered for each of the **Selected Zones**.



The **Zones** field is used to choose from a list of the Selected Zones for which flow observations will be entered.

The **Function** field lists the equation used in PEST to describe the different sources of flow contributing to the flow observation. This field automatically filled depending on the flow sources selected for the flow observation.

The **Flow IN** and **Flow OUT** lists contain all of the different sources of flow going **IN** to or **OUT** of the **Selected Zone**, respectively. For the example above, the flow observation is defined for the **Rivers zone** (all grid cells where a River boundary condition is defined). The flow observations indicate flow is entering the **Rivers zone** through **River leakage**.

The **Multiplier** field is used to indicate the relative contribution of each sources of flow to the **Selected zone**.

Occasionally, the way Zone Budget calculates flows may not correspond to the way the flows were measured in the field. For this case, the Observation table contains a means of summing the Zone Budget output such that the sum corresponds to the way the data was measured. Thus, each zone that you select from one of the lists, the zone and its

weight are added to the function line. Then PEST adds the Zone Budget output values according to the defined function prior to comparing the Zone Budget output to the observations.

3.8 Tools

The **Tools** menu item has the following options:

Cell Inspector	Displays the cell values for selected model parameters including grid co-ordinates, Kx, Ky, Kz, Ss, Sy, Head, and Concentration.
Annotation	Add lines, shapes, and text to the display screen.

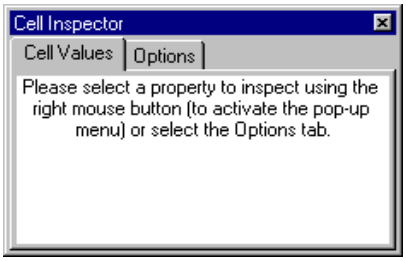
3.8.1 Cell Inspector

The Cell Inspector is used to inspect selected model parameter values on a cell-by-cell basis using the mouse to select the grid cell of interest. The model parameters that may be viewed in the Cell Inspector include:

- Grid Position (I, J, K number of grid cell)
- Model Position (X, Y, Z model co-ordinate values)
- World Position (X, Y, Z world co-ordinate values)
- Properties (Kx, Ky, Kz, Specific Yield, Specific Storage, Effective Porosity, Initial Head, and Initial Concentration values)
- Boundary Conditions (Boundary Condition name, Recharge, Evapotranspiration and Extinction Depth values)
- Output (Head and Concentration values)

Note: The Output data can only be viewed from the **Output** section

The Cell Inspector can be opened by selecting **Tools/Cell Inspector** from the top menu bar of either the **Input** or **Output** sections. The first time it is used in a model, the **Cell Inspector** window will be blank as shown in the following figure.

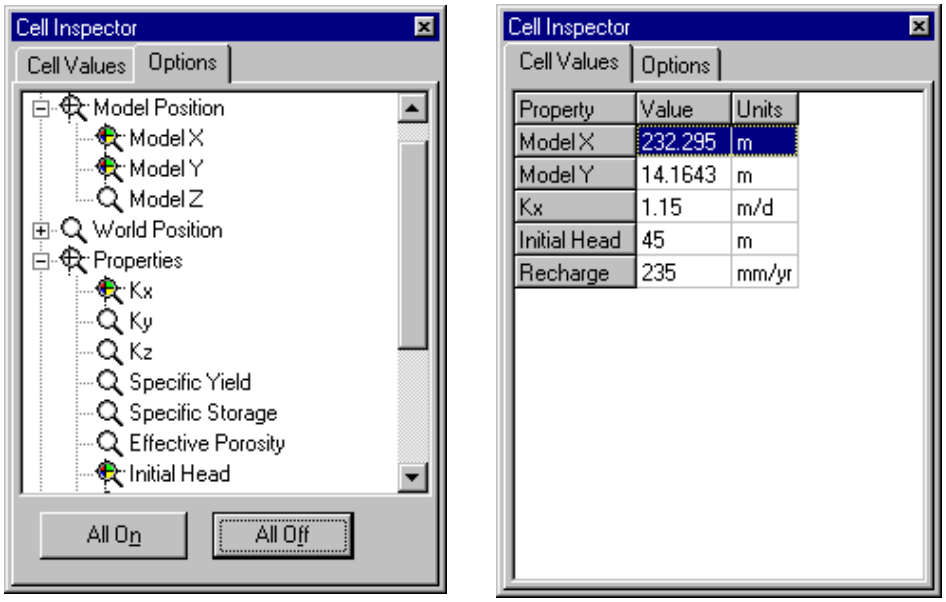

Cell Inspector
Cell Values
Options
Please select a property to inspect using the right mouse button (to activate the pop-up menu) or select the Options tab.

The **Cell Inspector** window has two tabs:

- The **Cell Values** tab displays the grid cell values of the selected parameters
- The **Options** tab is used to select the model parameters to data to view

The reason the **Cell Values** tab is blank is because it can be configured to display only the information of interest, and at this point no information has been selected. There are two ways to select the model parameters to display in the Cell Inspector:

- Right-click in the **Cell Values** tab and choose from the available options. A checkmark will appear next to the selected parameters.
- Click the **Options** tab and select the model parameters from the parameter groups. A colored cross-hair will appear in the magnifying glass icon next to selected parameters as shown in the following figure.



Once the parameters have been selected for viewing, switch to the **Cell Values** tab and move the cursor over the model domain. The values in the **Cell Inspector** window will be updated to reflect the parameter values in each grid cell.

To exit **Cell Inspector**, press the close button, in the top right-hand corner.

3.8.2 Annotate

Some basic graphics features have been included in Visual MODFLOW to add text, lines, arrows, and shapes to the model display screen.

To add some basic graphics to the model display area, choose **Tools/Annotate** from the top menu of the Input section and the following options appear on the left-hand toolbar:

[Add] Add an **Arrow**, **Rectangle**, **Circle**, **Text** or **Line** to the current layer, row, or column.

[Erase]	Erase a single graphic object or erase a group of object by stretching a box around the objects.
[Edit Single]	Edit the properties associated with selected graphic objects.
[Move Single]	Move selected graphic objects by clicking-and-dragging the object to a new location.

4

Run Section - Model Run Settings

This chapter describes the features, functionality and options in the **Run** section of the Visual MODFLOW interface. The **Run** section is where the model simulations are 'launched' (started) and it provides access to the run settings for the numeric engines chosen to run the flow, particle tracking, contaminant transport and parameter estimation simulations.

The top menu bar of the **Run** section contains the following menu items:

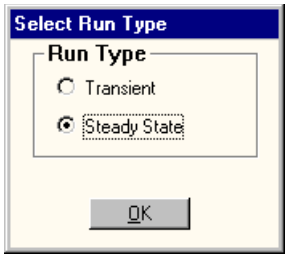
- **File**
- **MODFLOW***
- **MODPATH**
- **MT3D****
- **PEST**
- **Run**

* Depending on the numeric engine selected for running the flow simulation, the MODFLOW menu item may appear as MODFLOW-96 or MODFLOW-2000 (see section Groundwater Flow Numeric Engine on page 25).

** Depending on the numeric engine selected for running the contaminant transport simulation, the MT3D menu item may appear as MT3D1.5, MT3DMS, MT3D96, MT3D99, RT3D or RT3Dv2.5 (see section Mass Transport Numeric Engine on page 25).

Run Type: Steady-State or Transient

Upon entering the **Run** section of the Visual MODFLOW interface, the **Select Run Type** window appears as shown in the figure on the right.



If the **Steady-State** option is selected, Visual MODFLOW will prepare the data set for a steady-state simulation and will automatically use the data from the first time period of each boundary condition defined in Visual MODFLOW.

If the **Transient** option is selected, Visual MODFOW will prepare the data set for a transient simulation. During this process Visual MODFLOW

will automatically merge all of the different time period data defined for each pumping well and boundary condition into the stress period format required by the different versions of MODFLOW.

4.1 File

The **File** menu item is used for the following operations:

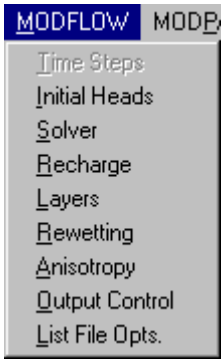
Save Save the current run settings.

Export… Export the model display to an Autocad (.DXF) file or an Enhanced Windows Metafile (.EMF).

Main Menu Return to the Main Menu of Visual MODFLOW.

4.2 MODFLOW Run Settings

As discussed previously, the MODFLOW menu item may appear as **MODFLOW-96** or **MODFLOW-2000** depending on which numeric engine has been selected to solve the flow simulation. **MODFLOW-2000** is the default selection for any new Visual MODFLOW models. The run settings available for both **MODFLOW-96** and **MODFLOW-2000** are as follows:



Time Steps Define the number of time steps and the time-step multiplier for each stress period (only available when the Transient run type option is selected).

Initial Heads Define the starting values for the initial head estimate.

Solver Choose a MODFLOW solver package.

Recharge Set recharge to be applied to either the top model layer, or to the uppermost active cells.

Layers Specify the layer types in the model, as described in the MODFLOW manual.

Rewetting Activate the wetting option of the BCF2 package and specify the rewetting variables.

Anisotropy Assign the anisotropy factor by layer.

Output Control Specify the times to save results and the formats.

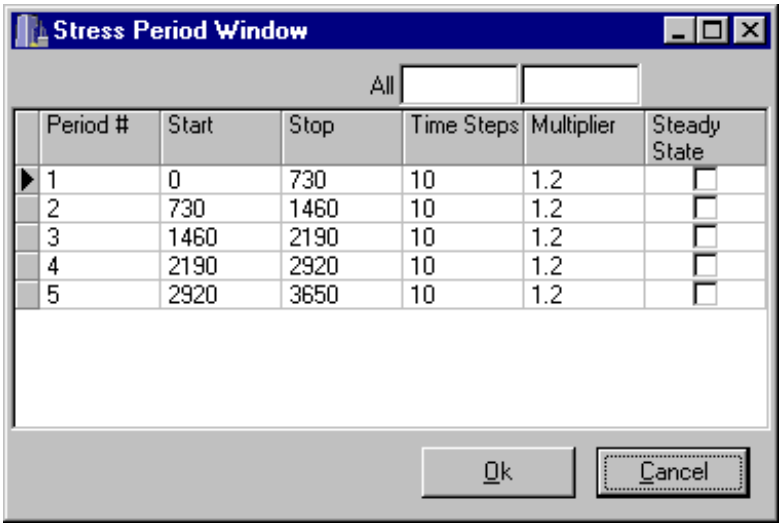
List File Opts. Specify the information and format to be written to the **.LST** file.

The settings each of these items are described in the following sections.

4.2.1 Time Steps

The **Time Steps** settings are only available when the **Transient** run type is selected. For transient simulations, Visual MODFLOW will automatically merge all of the different time period data defined for each pumping well and boundary condition into the stress period format required by MODFLOW. A stress period is defined as a time period in which all the stresses (boundary conditions, pumping rates, etc.) on the system are constant. Unfortunately, the data collected for each modeling site is rarely synchronized in terms of stress periods, so Visual MODFLOW merges the time schedules for all pumping wells and boundary conditions to determine the length of each stress period for a transient simulation. As a result, the user cannot directly modify the number of stress periods or the length of each stress period.

The **Time Steps** settings are defined in the **Stress Period Window** as shown in the following figure. This window is used to define the number of **Time Steps** in each stress period and the time step **Multiplier** used to increment each time step (as shown in the following figure).



The **Period #** column indicates the stress period number while the **Start** and **Stop** columns indicate the start time and stop time, respectively, for each stress period.

Each stress period is divided into a user-defined number of **Time Steps** whereby the model will calculate the head solution at each time step.

The time step **Multiplier** is the factor used to increment the time step size within each stress period (i.e. it is the ratio of the length of each time step to that of the preceding time step).

A time step **Multiplier** value greater than 1 will produce smaller time steps at the beginning of a stress period resulting in a better representation of the transient changes

of the flow field. Thus increasing the number of time steps in a simulation may result in smoother head or drawdown versus time curves.

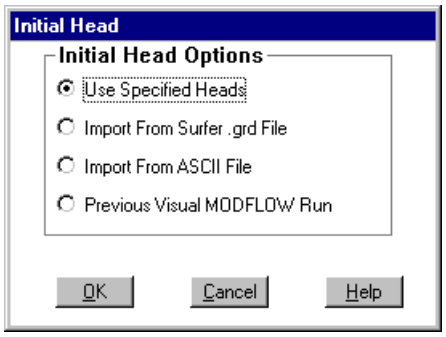
The **Steady-State** column indicates if the **Stress Period** is transient or steady-state. This option is only available if MODFLOW-2000 is selected as the numeric engine for the flow model. MODFLOW-2000 allows individual stress periods in a single simulation to be either transient or steady state instead of requiring the entire simulation to be either steady state or transient. Steady-state and transient stress periods can occur in any order. Commonly the first stress period is steady state and produces a solution that is used as the initial condition for subsequent transient stress periods.

4.2.2 Initial Heads

In order to start solving the flow simulation MODFLOW requires an initial "guess" for the head values in the model. A good initial guess for the starting heads of the simulation can reduce the required run time significantly. A bad initial head estimate can cause non-convergence of the solution or n result in unnecessary dry cells if the Cell Rewetting package is not turned on.

Initial head values are also used to calculate the drawdown values, as measured by the difference between the starting head and the calculated head.

The **Initial Heads** run settings provides four options for defining the initial head estimate for the simulation:



- **Use Specified Heads** will use the initial heads specified by the user in the Input section of Visual MODFLOW. If no initial heads were specified, Visual MODFLOW will automatically set all initial heads equal to the highest head value defined by a head dependent boundary condition.
- **Import from Surfer .grd File** will use data from selected Surfer file(s) to calculate the initial heads for each layer of the model. See the section Importing Initial Heads on page 163.
- **Import from ASCII File** will use data from selected ASCII file(s) to calculate the initial heads for each layer of the model. See the section Importing Initial Heads on page 163.
- **Previous Visual MODFLOW Run** will use a binary format heads file (.HDS) from a previous Visual MODFLOW simulation as the initial head values for the current simulation. The selected .HDS file must have the same number of rows, columns and layers as the current model.

When importing from a **Previous Visual MODFLOW Run**, if the model was run in transient mode, you may select from the list of times and timesteps. If the model was run in steady-state mode, you can only select the steady-state time of 1. This is very useful when trying to calibrate a model or perform a sensitivity analysis, as it provides the model with an initial guess that will closely resemble the solution. If the grid has been refined, the old ***.HDS file cannot be used.

Importing Initial Heads

Initial heads can be imported in both the **Input** section and the **Run** section of Visual MODFLOW. As discussed in Chapter 3, the advantage to importing the initial heads in the **Run** section is the values are exact because it is not necessary to calculate values for the constant value initial head property zones. The disadvantage to importing in the **Run** section is you are unable to view the distribution of initial head values before running the model.

In the **Run** section Visual MODFLOW can import initial heads data from:

- **ASCII** files (.TXT) in world or model co-ordinate system
- **Surfer** files (.GRD) in world or model co-ordinate systems

The ASCII file (.TXT) must be saved in comma or tab delimited format with the following data structure:

```
X-Coordinate, Y-Coordinate, Initial Head Value
```

For example:

```
1120, 2352, 34
3392, 4491, 36
2892, 2531, 29
3590, 1803, 32
```

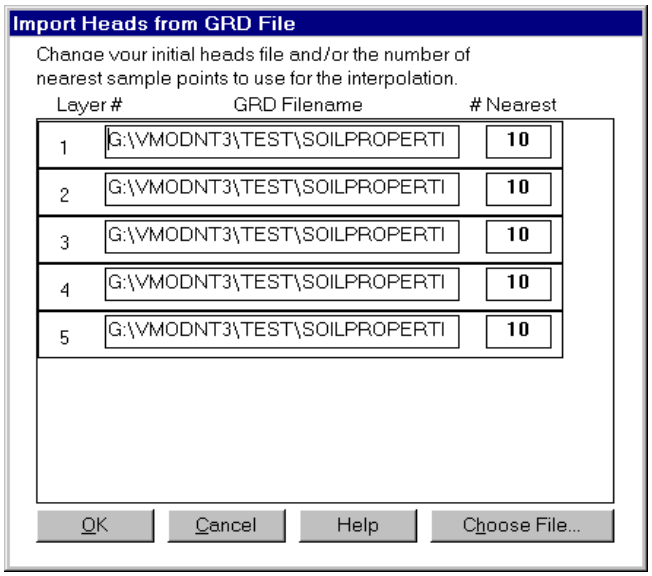
No header information or column titles are allowed and the coordinate locations for the data points must be within the model domain. If different initial head values are required for different sets of layers in the model, then separate ASCII text files must be prepared for each set of model layers.

The Surfer Grid files must be saved in binary format and the majority of the grid domain must correspond with the model domain. If different initial head values are required for different sets of layers in the model, then separate Surfer Grid files must be prepared for each set of model layers

Visual MODFLOW uses an inverse distance interpolation method to calculate the head value for the center of each grid cell.

To import initial heads from an **ASCII** file or a **Surfer** file,

- Choose the source file type from the **Initial Heads** dialog and click **[OK]**.
- Select the source file for the first layer of the model and click **[Open]**.
- An **Import Initial Head** dialog will appear with the selected source file applied for each layer of the model (see figure below).
- To use a different source file for different layers, click in the target layer and use the **[Choose File]** button to select the appropriate file for each layer.
- Enter the appropriate number of **Nearest Neighbors** (nearest data points) to use during the interpolation procedure for each layer of the model.
- Click **[OK]** to interpolate the initial heads data to the model grid and import the array into Visual MODFLOW.



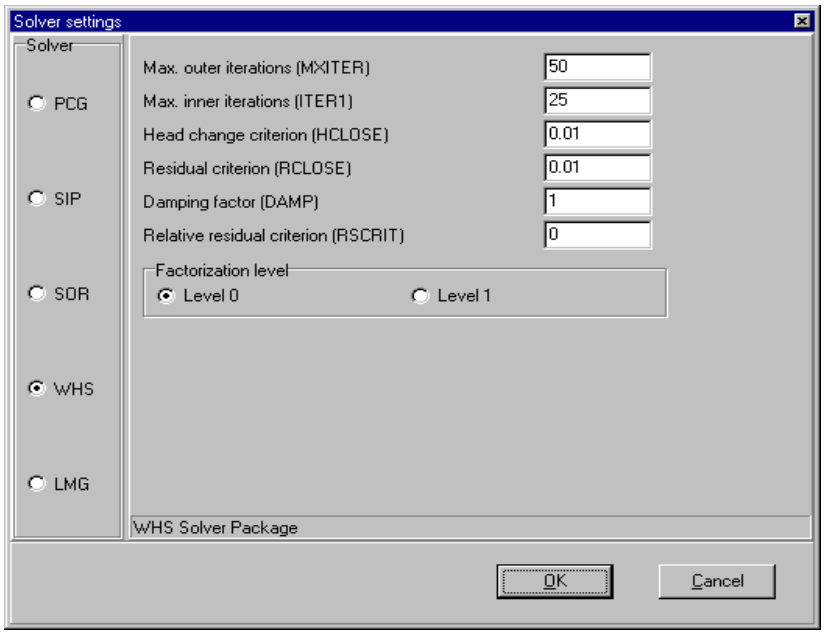
4.2.3 Solver Settings

Visual MODFLOW comes with a choice of different solvers to use in solving the numerical equations for the flow simulation:

- SSOR - Slice-Successive Over-Relaxation
- SIP - Simply Implicit Procedure
- PCG2 - Preconditioned Conjugate Gradient
- LMG - Algebraic Multigrid (only available with MODFLOW-2000)
- WHS - Bi-Conjugate Gradient Stabilized

These solvers and their individual settings can be accessed by selecting **MODFLOW/ Solver** from the **Run** section of Visual MODFLOW. A **Solver Selection** window will appear as shown in the following figure with a dropdown picklist for choosing the

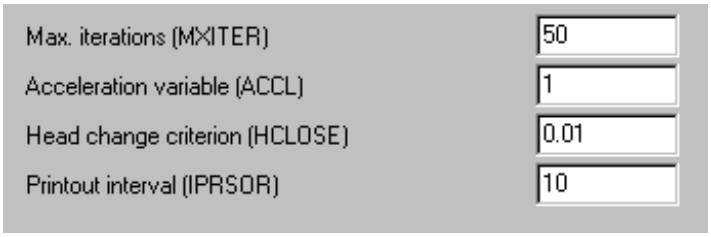
desired **Solver** and a listing of the settings for the selected **Solver**. Each new Visual MODFLOW model will be set to use the WHS Solver by default.



The following sections provide a detailed description of how each solver works and the associated parameter settings.

Slice-Successive Overrelaxation Package (SOR)

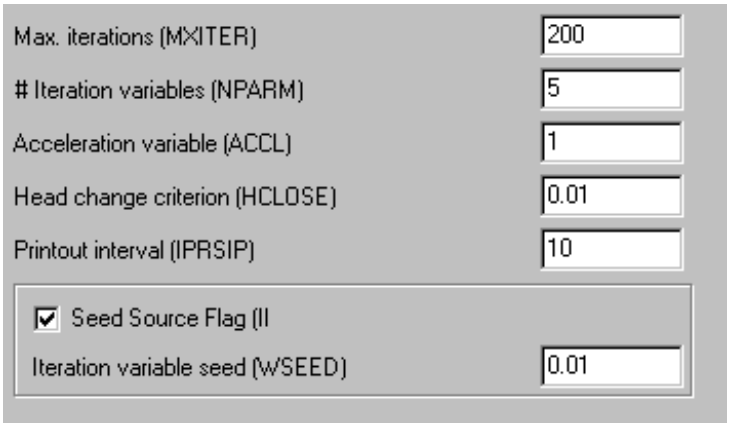
Slice-Successive Over-Relaxation is a method for solving large systems of linear equations by means of iteration. It is implemented in the SOR Package by dividing the finite difference grid into vertical slices, and grouping the node equations into discrete sets, each set corresponding to a slice. In every iteration, these sets of equations are processed in turn, resulting in a new set of estimated head values for each slice. As the equations for each slice are processed, they are first expressed in terms of the change in computed head between successive iterations. The set of equations corresponding to the slice is then solved directly by Gaussian elimination, treating the terms for adjacent slices as known quantities. The values of head change computed for the slice are then each multiplied by an acceleration factor, T, generally taken between 1 and 2; the results are taken as the final values of head change in that iteration for the slice. This procedure is repeated for each slice in sequence until all of the slices in the three-dimensional array have been processed, thus completing a domain iteration. The entire sequence is then repeated, until the differences between the head values computed in successive iterations is less then the chosen criterion at all nodes in the mesh. The SOR Package is described in Chapter 13 of the MODFLOW manual.



- **Maximum Number of Iterations:** [Default = 50] This parameter provides an upper limit on the number of iterations to be performed. The maximum number of iterations will only be used if a convergent solution is not reached beforehand. 50 iterations should be more than adequate for most problems. However, if the maximum number of outer iterations is reached and an appropriate mass balance error is not achieved, this value should be increased.
- **Acceleration Factor:** [Default = 1] The acceleration factor controls the magnitude of head changes between iterations. The acceleration factor must be positive. Values larger than one will result in larger head changes between iterations; the solution may be approached faster but it may also overshoot the solution more easily. Values less then one will result in smaller head changes, thus, requiring more iterations to reach a solution.
- **Head Change Criterion for Convergence:** [Default = 0.01] After every iteration is completed, the solver checks for the maximum change in the solution at every cell. If the maximum change in the solution is below a set convergence tolerance (set here in the working units of feet or metres) then the solution has converged and the solver stops, otherwise a new iteration is started. A solution accurate to 0.01 [ft or m] will normally be sufficient for most problems unless the maximum head change throughout the modeled domain is smaller than 1 foot or metre. If an appropriate mass balance is not achieved and the number of iterations is less than the maximum, this value can be decreased by an order of magnitude.
- **Printout Interval:** [Default =10] The printout interval indicates the number of iterations between which head information is written to the listing (.LST) file.

Strongly Implicit Procedure Package (SIP)

The **Strongly Implicit Procedure**, also known as **SIP**, is a method for solving a large system of simultaneous linear equations by iteration. The advantage of the SIP solver is that it is very stable and generally converges to a solution but often very slowly. It is not as fast as the PCG method, but it requires less memory to compute the final solution. Because each equation involves up to seven unknown values of head, and because the set of unknown values changes from one equation to the next throughout the grid, the equations for the entire grid must be solved simultaneously at each time step. This package is described in Chapter 12 of the MODFLOW manual.



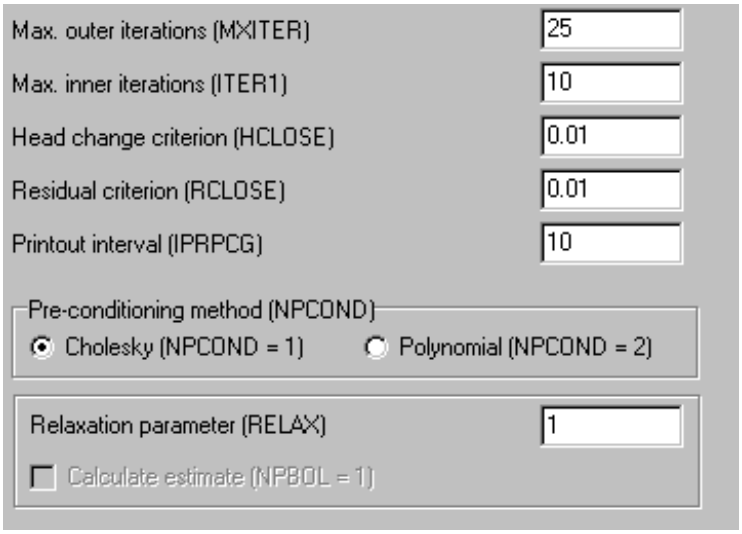
The solver parameters for the SIP method are described below:

- **Maximum Number of Iterations:** [Default = 200] This is the upper limit on the number of iterations to be performed. The maximum number of iterations will only be considered if a convergent solution is not reached beforehand. Two hundred iterations should be more than adequate for most problems. However, if the maximum number of iterations is reached and an appropriate mass balance error is not achieved, this value should be increased.
- **Number of Iteration Parameters:** [Default = 5] The finite difference equations describing the groundwater flow system can be put into matrix form as [A]{h}={q}. Where [A] is the coefficient matrix, {h} is the heads array and {q} is the flux array. The number of iteration parameters indicates the number of parameters that will be used to transform the initial coefficient matrix [A] to a similar matrix that can be decomposed into two lower and upper triangular matrices [L] and [U] respectively. The default value of 5 is generally sufficient.
- **Acceleration Factor:** [Default = 1] The acceleration factor controls the magnitude of head change between iterations. The acceleration factor must be positive. Values larger than one will result in larger head changes between iterations; the solution may be approached faster but it may also overshoot the solution more easily. Values less then one will result in smaller head changes, thus, requiring more iterations to reach a solution.
- **Head Change Criterion for Convergence:** [Default = 0.01] After every iteration is completed, the solver checks for the maximum change in the solution at every cell. If the maximum change in the solution is below a set convergence tolerance (set here in the working units of feet or metres) then the solution has converged and the solver stops, otherwise a new iteration is started. A solution accurate to 0.01 [ft or m] will normally be sufficient for most problems unless the maximum head change throughout the modeled domain is smaller than one foot or metre. If an appropriate mass balance is not achieved and the maximum number of iterations is not reached, this value can be decreased by an order of magnitude.

- **Printout Interval:** [Default = 10] The printout interval indicates the number of iterations in between which head information is written to the listing (.LST) file.
- **User Seed Value:** [Default = 0.01] There are two options: either the user can enter the seed or the seed will be calculated at the start of the simulation from problem parameters. The iteration parameter 'seed' is used as a basis for determining the sequence of w values. The w multiplies each term on the right side of the equation; and must be cycled through a series of values in successive iterations to achieve satisfactory rates of convergence. The more strongly diagonal the coefficient matrix, the less important the choice of seed will be.

Preconditioned Conjugate-Gradient Package (PCG2)

PCG2 uses the preconditioned conjugate-gradient method to solve the simultaneous equations produced by the model. Linear and non-linear flow conditions may be simulated. PCG2 includes two preconditioning options: modified incomplete Cholesky preconditioning, which is efficient on scalar computers; and polynomial preconditioning, which requires less computer storage and, with computer specific modifications, is most efficient on vector computers. Convergence of the solver is determined using both the head-change and residual criteria. Non-linear problems are solved using the Picard iterations. The PCG2 Package is described in Water-Resources Investigations Report 90-4048 of the USGS, (by Mary Hill, 1997), which is included in the reference manual.



The PCG2 solver works on a two-tier approach to a solution at one time step. Outer iterations are used to vary the preconditioned parameter matrix in an approach toward the solution. An outer iteration is where the hydrogeologic parameters of the flow system are updated (i.e., transmissivity, saturated thickness, storativity) in the

preconditioned set of matrices. The following is a description of the solver parameters for the PCG method:

- **Maximum Number of Outer (non-linear) Iterations:** [Default = 25] This parameter provides an upper limit on the number of outer iterations to be performed. The maximum number of iterations will only be used if a convergent solution is not reached beforehand. Twenty-five iterations should be more than adequate for most problems. However, if the maximum number of outer iterations is reached and an appropriate mass balance error is not achieved, this value should be increased.
- **Maximum Number of Inner Iterations:** [Default = 10] This parameter provides an upper limit on the number of inner iterations to be performed. This number of iterations will only be used if a convergent solution for the current set of matrices in the "outer" iteration is not reached beforehand. Ten inner iterations should be more than adequate for most problems. More than ten iterations will not usually improve the solution, as the solution is updated again when it returns to the outer iterations.
- **Head Change Criterion for Convergence:** [Default = 0.01] After all outer iterations have completed the solver checks for the maximum change in the solution at every cell. If the maximum change in the solution is below a set convergence tolerance (set here in the working units feet or metres) then the solution has converged and the solver stops, otherwise a new outer iteration starts.
- A solution accurate to 0.01 [ft or m] will normally be sufficient for most problems unless the maximum head difference across the modeled domain is smaller than one foot or metre. If an appropriate mass balance is not achieved and the number of inner and outer iterations are within the maximums declared above, this value can be decreased by an order of magnitude, e.g. 0.001.
- **Residual Criterion for Convergence:** [Default = 0.01] While the head change criterion is used to judge the overall solver convergence, the residual criterion is used to judge the convergence of the inner iterations of the solver. If the maximum absolute value, of the residual at all nodes, is less than the tolerance specified here (units of length^3/time) then the solver will proceed to the next outer iteration.

  Normally the head change criterion and the residual criterion are equal. A value of 0.01 ft^3/s or m^3/s is usually sufficient (default). However, if you notice that only a few inner iterations are being performed for all outer iterations, and an appropriate mass balance is not achieved, this value can be decreased by one or more orders of magnitude.

  > **Note:** The residual criterion is unit dependent. The default value of 0.01 is sufficient if your length units are feet or metres and your time units are seconds. If your time units are not seconds you should multiply the default value by the number of seconds in your time unit (e.g. use a residual criterion of 864, if your time unit is days.

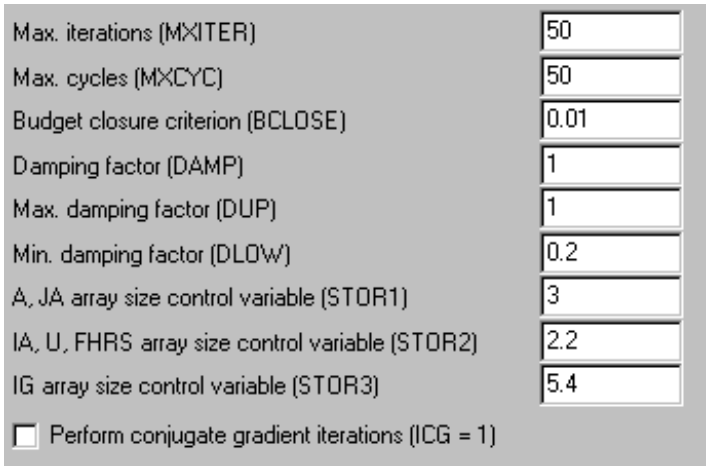
- **Printout Interval:** [Default =10] The printout interval indicates the number of iterations in between which head information is written to the listing (.LST) file.

Link-Algebraic Multigrid Solver (LMG)

Visual MODFLOW supports the Link-Algebraic Multigrid (LMG) Package provided with MODFLOW-2000 and documented in the U.S. Geological Survey Open-File Report 01-177 (Mehl and Hill, 2001). The LMG Package links MODFLOW-2000 with an advanced technique for solving matrix equations, the freeware algebraic multigrid (AMG) solver produced by the GMD - German National Research Center for Information Technology. The LMG Package has some distinct advantages over other solvers available with MODFLOW-2000 for problems with large grids (more than about 40,000 cells) and (or) a highly variable hydraulic-conductivity field. Testing conducted by the U.S. Geological Survey indicate that execution times using the AMG solver may be 2 to 25 times faster than execution times using MODFLOW's PCG2 Package with the modified incomplete Cholesky pre conditioner. The drawback to the AMG method used in the LMG Package is that is may require 3 to 8 times more memory than PCG2.

The advantages of multigrid methods over the other iterative solvers mentioned are (1) the effectiveness of the multigrid solver is not as dependent on the initial head distribution, and (2) for many problems of interest, the rate of convergence scales approximately linearly with the size of the domain, unlike the other solvers where the rate of convergence increases nonlinearly (Demmel, 1997, p. 277).

There are a number of user-defined solver settings which can influence the speed and effectiveness of the AMG solver. The following description of these settings are taken from the U.S. Geological Survey Open-File Report 01-177 (Mehl and Hill, 2001).



- **Max. iterations (MXITER):** [Default = 50] **MXITER** is the maximum number of times that the AMG routines will be called to obtain a solution. **MXITER** is never less than 2 and rarely more than 50. MXITER often equals 2 when the problem is linear (all layers are confined, and no boundary conditions are nonlinear; the Evapotranspiration, Drain, and River Packages, for example, produce nonlinear boundary conditions). For nonlinear problems, **MXITER** generally is 50 or less; however values near 50 and sometimes even larger are needed for more severely nonlinear problems.
- **Max. cycles (MXCYC)**: [Default = 50] For each call to the solver, AMG cycles through one or more sequences of coarsening and refinement. The solver is limited to a maximum of **MXCYC** cycles per call to the solver. For most problems, convergence for each iteration is achieved in less than 50 cycles, so that generally **MXCYC** can be less than 50. For highly nonlinear problems, however, better performance may be achieved by limiting the solver to a small number of cycles and increasing the maximum number of iterations (**MXITER**). This prevents the solver from needlessly finding very accurate solutions at early iterations of these highly nonlinear problems.
- **Budget closure criterion (BCLOSE)**: [Default = 0.01] The AMG routine is called iteratively until the convergence criterion **BCLOSE** is met or the number of iterations has exceeded **MXITER**. A convergence criterion value that is too large can be detected in MODFLOW-2000 by unacceptably large global ground-water flow budget errors, sensitivity errors, or both. If such problems exist, **BCLOSE** should be decreased. Typically, decreasing **BCLOSE** by one order of magnitude will decrease the global budget error by about one order of magnitude.
- **Damping factor (DAMP)**: [Default = 1] The damping factor can be used to restrict the head change from one iteration to the next, which commonly is useful in very nonlinear problems. **DAMP** makes the solution change slowly, thus avoiding spurious deviations prompted by nonlinear effects at intermediate solutions. Values of **DAMP** less than 1.0 restrict the head change (under-relaxation), while values greater than 1.0 accelerate the head change (over-relaxation). For linear problems, no damping is necessary, and **DAMP** should be set equal to 1.0. For non-linear problems, restricting the head change (**DAMP** < 1.0) may be necessary to achieve convergence, and values of **DAMP** between 0.5 and 1.0 are generally sufficient.

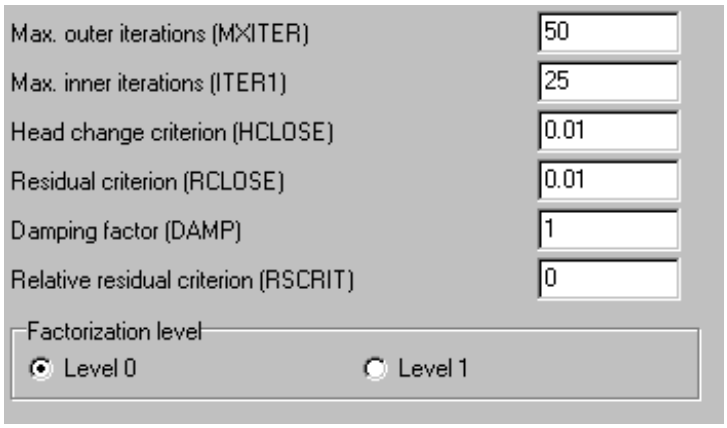
  For some nonlinear problems, imposing a fixed value of DAMP for every iteration can hinder convergence. One remedy for this condition is to adjust the amount of damping depending on how the head solution progresses. The LMG Package provides two adaptive damping strategies; (1) Cooley's method with Huyakorn's modification; and (2) the relative reduced residual method. These methods are described in detail in the U.S. Geological Open-File Report 01-177. A **DAMP** value of -1 will utilize the first method, and a **DAMP** value of -2 will utilize the second method.

- **Max. damping factor (DUP)**: [Default = 1] The upper limit for **DAMP** when an adaptive damping strategy is used.
- **Min. damping factor (DLOW)**: [Default = 0] The lower limit for **DAMP** when an adaptive damping strategy is used.
- **Perform conjugate gradient iterations (ICG)**: [Default = 0] In some cases, AMG can perform poorly as a result of a small number of error components that are not reduced during the AMG cycling. A few iterations of a conjugate gradient solver can often reduce these error components and thus help convergence (Cleary and others, 2000). In these cases, the parameter **ICG** can be set to 1 to perform conjugate gradient iterations at the end of each multigrid cycle. Activating this option can decrease execution times for some problems, but it will also increase the amount of memory used by the solver.
- **A, JA array size control variable (STOR1)**: [Default = 3] See U.S. Geological Survey Open-File Report 01-177 for details.
- **IA, U, FHRS array size control variable (STOR2)**: [Default = 2.2] See U.S. Geological Survey Open-File Report 01-177 for details.
- **IG array size control variable (STOR3)**: [Default = 5.4] See U.S. Geological Survey Open-File Report 01-177 for details.

WHS Solver for Visual MODFLOW (WHS)

The **WHS Solver** uses a Bi-Conjugate Gradient Stabilized (Bi-CGSTAB) acceleration routine implemented with Stone incomplete decomposition for preconditioning of the groundwater flow partial differential equations. This solver, as all iterative solvers, approaches the solution of a large set of partial differential equations iteratively through an approximate solution. Because the matrix equation for groundwater flow is initially "ill-conditioned", effective pre-conditioning of these matrices is necessary for an efficient solution. Two "levels" of factorization are available with the WHS solver. While convergence of the solver requires fewer iterations with a factorization level of 1, the memory required to run the solver increases with this factorization level. Also, the work per iteration increases with the level 1 factorization such that the total solution time may not be less than the solution time using level 0 factorization.

The WHS solver works on a two-tier approach to a solution at one time step. Outer iterations are used to vary the factorized parameter matrix in an approach toward the solution. An outer iteration is where the hydrogeologic parameters of the flow system are updated (i.e., transmissivity, saturated thickness, storativity) in the factorized set of matrices. Different levels of factorization allow these matrices to be initialized differently to increase the efficiency of solution and model stability. Inner iterations are used to iteratively solve the matrices created in the outer iteration.



- **Maximum Number of Outer (non-linear) Iterations:** [Default = 50] This parameter provides an upper limit on the number of outer iterations to be performed. The maximum number of iterations will only be used if a convergent solution is not reached beforehand. Fifty iterations should be more than adequate for most problems. However, if the maximum number of outer iterations is reached and an appropriate mass balance error is not achieved, this value should be increased.
- **Maximum Number of Inner Iterations:** [Default = 25] This parameter provides an upper limit on the number of inner iterations to be performed. This number of iterations will only be used if a convergent solution for the current set of matrices in the "outer" iteration is not reached beforehand. Twenty-five inner iterations should be more than adequate for most problems. However, if the maximum number of inner iterations was used for all outer iterations and an appropriate mass balance error was not achieved, this value can be increased.
- **Head Change Criterion for Convergence:** [Default = 0.01] After every outer iteration is completed, the solver checks for the maximum change in the solution at every cell. If the maximum change in the solution is below a set convergence tolerance (set here in the working units of feet or metres) then the solution has converged and the solver stops, otherwise a new outer iteration is started. A solution accurate to 0.01 [ft or m] will normally be sufficient for most problems unless the maximum head change throughout the modeled domain is smaller than 1 foot or metre. If an appropriate mass balance is not achieved and the number of inner and outer iterations is within the maximums, this value can be decreased by an order of magnitude.
- **Residual Criterion for Convergence:** [Default = 0.001] While the head change criterion is used to judge the overall solver convergence, the residual criterion is used to judge the convergence of the inner iterations of the solver. If the change in successive inner iterations is less than the tolerance specified here (in working units of feet or metres), then the solver will proceed with the

next outer iteration. This residual criterion for convergence of 0.001 should be appropriate for most problems. However, if you notice that only a few inner iterations are being performed for every outer iteration and an appropriate mass balance is not achieved, this parameter value can be decreased by one or more orders of magnitude.

- **Dampening Factor for the Outer Iterations:** [Default = 1] This factor allows the user to reduce (dampen) the head change calculated during each successive outer iteration. For most "well posed" and physically realistic groundwater flow problems, the dampening factor of one will be appropriate. This parameter can be used to make a non-convergent (oscillating or divergent) solution process more stable such that a solution will be achieved. This is done by decreasing the dampening factor to a value between 0 and 1 (only rarely < 0.6). This parameter is similar to "acceleration parameters" used in other solvers.
- **Relative Residual Criterion:** [Default = 0] This parameter provides another method of checking for convergence of the inner iteration. This method compares the residual from the most recent inner iteration to the residual from the initial inner iteration. Once the most recent inner iteration residual is below the initial inner iteration residual times the relative residual criterion, the current outer iteration is completed and a new outer iteration will be started.
- **Factorization Level:** [Default = 1] There are two levels of factorization, 0 and 1. **Level 0** requires more outer iterations but less memory. **Level 1** requires fewer outer iterations but more memory.

4.2.4 Recharge Settings

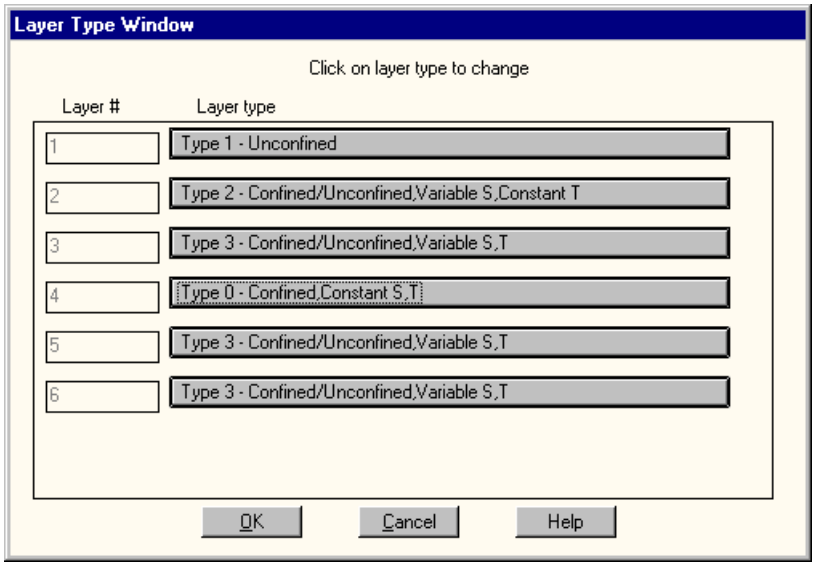
In Visual MODFLOW the Recharge zone distribution can only be applied while viewing Layer 1. However, if some cells in the top layer become dry during the course of the simulation, or if some cells in the top layer are designated as no-flow cells, the MODFLOW program allows the recharge to be applied to the grid cell in the upper most active (wet) layer in the model. The **Recharge** settings in Visual MODFLOW are described below.

- **Recharge is only applied to the top grid layer:** If any grid cells in Layer 1 are dry, or if they are designated as no-flow cells, the recharge values assigned to these grid cells will NOT be carried down to the underlying active (wet) grid cells. In this case, the inactive or dry cells act like an impermeable barrier to the recharge.
- **Recharge is applied to the highest active cell in each vertical column:** If any grid cells in Layer 1 are dry, or if they are designated as no-flow cells, the recharge values assigned to these grid cells will be carried down to the upper most active (wet) grid cell in the same vertical column of grid cells.

Note: A constant head boundary condition always intercepts recharge and prevents deeper infiltration.

4.2.5 Layer Type Settings

The **Layers** run settings are used to specify the **Layer Type** for each layer of the model grid (see following figure). The **Layer #** column has one row for each layer of the model grid, while the **Layer Type** column lists the specified Layer Type for each model layer. MODFLOW has four different Layer Types to choose from as described below.



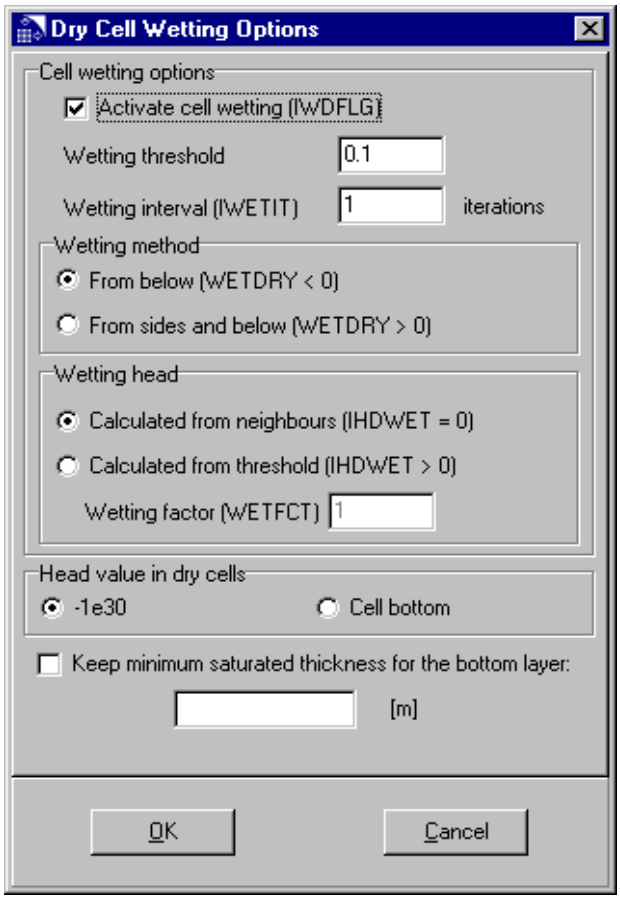
- **Type 0 Confined**: Transmissivity and storage coefficients of the layer are constant for the entire simulation.
- **Type 1 Unconfined:** Transmissivity of the layer varies and is calculated from the saturated thickness and hydraulic conductivity. The storage coefficient is constant; valid only for layer 1.
- **Type 2 Confined/Unconfined**: Transmissivity of the layer is constant. The storage coefficient may alternate between confined and unconfined values.
- **Type 3 Confined/Unconfined**: Transmissivity of the layer varies. It is calculated from the saturated thickness and hydraulic conductivity. The storage coefficient may alternate between confined and unconfined values. Vertical leakage from above is limited if the aquifer becomes desaturated.

The **Layer Type** can be toggled to a different select by simply clicking on the current selection.

4.2.6 Re-wetting Settings

The original USGS MODFLOW did not allow cells in unconfined layers to become re-saturated if the head dropped below the bottom elevation of the grid cell during the course of the simulation or during the solution iterations. Instead, these cells were simply made inactive for the remainder of the simulation. However, the USGS later extended the Block-Centered-Flow package (BCF2) to allow for the rewetting of these "dry" cells during a transient simulation. While this represented a major advancement for more accurate representations of water table aquifers, it also causes the solution to be much more unstable in some situations. More detailed information on the cell wetting and the BCF package can be found in the MODFLOW Packages Reference Manual.

The **Re-wetting** settings may be accessed by selecting MODFLOW/Re-wetting from the top menu bar of the Run section. A **Dry cell wetting options** window will appear as shown in the following figure and described below.



- **Activate cell wetting (IWDFLG)** is used to indicate if the wetting capability is active (**IWDFLG = 1**) or inactive (**IWDFLG = 0**).
- **Wetting threshold** is used to determine if the dry cell needs to be wetted. For a dry cell to become wet, the head in the adjacent grid cell(s) must be greater than the elevation of the bottom of the dry cell plus the **Wetting threshold** value.
- **Wetting interval (IWETIT)** indicates how often MODFLOW attempts to wet the dry cells detected during the course of the solution iterations. For example, if **IWETIT = 2**, cell wetting would be attempted at every second iteration. If a model with dry cells is having problems converging to a solution, it may be a result of oscillations due to drying and re-wetting of grid cells in sensitive regions of the model. Setting a large cell wetting interval value may help the solution to converge by allowing the heads in neighboring cells to get closer to a better solution before wetting the dry cells.

Wetting Methods

The wetting of a dry cell is triggered by the head values in adjacent grid cells (see **Wetting threshold** above). The **Wetting method** frame has two options for determining the adjacent grid cells to use for determining whether the dry cell should be wetted.

- **From below (WETDRY < 0)** will use only the head in the grid cell directly below the dry cell to determine if the dry cell should be wetted. This option is generally more stable and is particularly good when the adjacent horizontal cells are poor indicators of whether a cell should become wet (e.g. areas with steep vertical gradients and variable bottom elevations).
- **Wet cells from side and below (WETDRY > 0)** will used the head in all four adjacent grid cells and the grid cell directly below the dry cell to determine if the dry cell should be wetted. This option is useful in situations where a dry cell is located above a no-flow cell, such that it cannot re-wet from below. It is also applicable for one-layer models where there are no cells below. However, this method can cause some problems in multi-layer models whereby dry cells occur beneath wet cells.

Wetted Head

When a dry cell is wetted, the new head may be calculated using one of two methods:

- **Calculated from neighbors**

  $$\textbf{Head} = \textbf{Z}_{\textbf{bot}} + \textbf{Wetting factor} * (\textbf{Neighbouring head} - \textbf{Z}_{\textbf{bot}})$$

- **Calculated from threshold**

  $$\textbf{Head} = \textbf{Z}_{\textbf{bot}} + \textbf{Wetting factor} * (\textbf{Wetting threshold})$$

Where $\textbf{Z}_{\textbf{bot}}$ is the elevation of the bottom of the current cell.

Generally, the first equation is thought to be more reasonable since the cell's new head is varied according to the head in the neighbouring cell, which caused it to become wet. However, in situations where MODFLOW is over-estimating head changes during iterations, this equation may cause non-convergence. The second equation can then be used to attempt a more stable solution.

Setting Head Values in Dry Cells

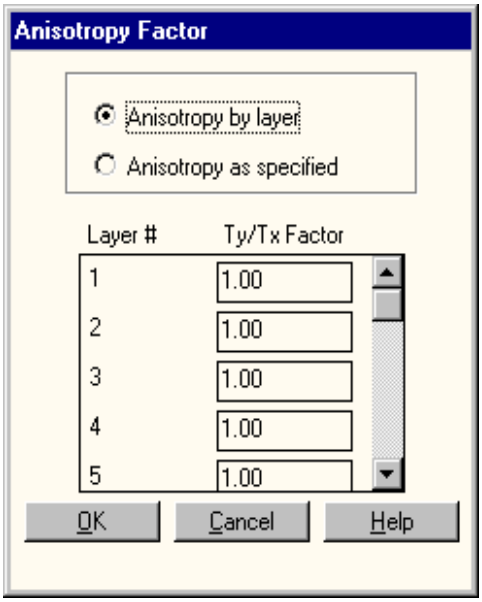
Each dry cell is assigned a default head value as a flag to indicate it is dry. This value is typically a very large negative number (e.g. -1.0e-30). However, the presence of large negative head values in dry cells may cause problems for parameter estimation simulations because this large negative value may be used to calculate the calibration residual (calculated head - observed head) at a grid cell that has become dry during one of the PEST iterations. In this case, it is more appropriate to assign the head value in dry cells equal to the cell bottom elevation to avoid this problem.

Hints For Using Dry Cell Wetting

Cell re-wetting often promotes a non-converging or unstable solution, which may be indicated by cells cycling between wet and dry. If this happens we recommend you try the following:

- Make inactive any cells that you know should never become wet.
- Increase the **Wetting threshold** value. This makes it more difficult for a cell to be wetted and therefore helps stop MODFLOW from repeatedly turning a cell on and then off again. However, the solution may become less accurate since cells that should become wet might stay dry.
- Modify the **Wetting factor** value. This will increase or decrease the new head in cells which are wetted.
- Change the **Wetting method** that controls cell wetting.
- Change the **Wetted head** option that calculates the new head in the wetted cell.
- Try using the SIP or PCG solver and modifying the solver parameters.
- For steady-state solutions start with good initial estimates of final conditions. This will provide good indications of which cells should be wet and dry and therefore conversions of cells between wet and dry will be minimized.

4.2.7 Anisotropy Settings



Horizontal anisotropy is the ratio of transmissivity or hydraulic conductivity along a column to its component value along each row. The **Anisotropy** settings in Visual MODFLOW may be accessed in the **Run** section by selecting **MODFLOW/ Anisotropy** from the top menu bar. The following **Anisotropy Factor** window will provide two choices for determining how the anisotropy is calculated for the model.

- **Anisotropy by layer**
- **Anisotropy as specified**

The **Anisotropy by layer** option uses the anisotropy ratio (**Ty/Tx Factor**) specified for each layer of the model (see figure on right) and the Kx values specified in each grid cell to calculate the Ky or Ty values for each grid cell. Selecting **Anisotropy by layer** will not remove the original values for Ky, but will instead calculate them during the translation of Visual MODFLOW file formats to MODFLOW input data file formats. By default each new simulation will be set to use the **Anisotropy by layer** option.

The Anisotropy as specified option will use the Kx and Ky values defined for each property zone. This feature allows spatially variable anisotropy within a layer as opposed to the **Anisotropy by layer** option which applies a single anisotropy ratio (**Ty/ Tx Factor**) for the entire layer. A more in depth discussion of spatially variable anisotropy can be found in Kladisa, 1997.

4.2.8 Output Control Settings

Each MODFLOW simulation can produce three binary output files and one ASCII output file:

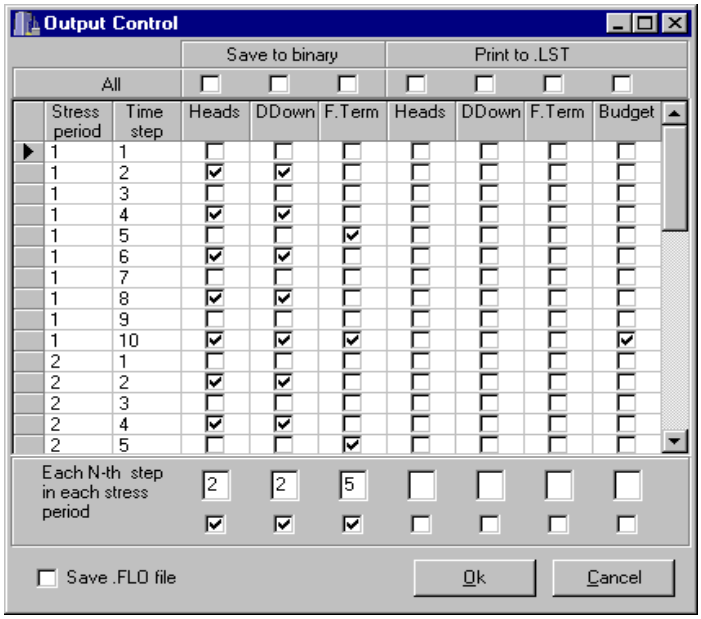
- Binary head file (*modelname*.HDS)
- Binary drawdown file (*modelname*.DDN)
- Binary flow file (*modelname*.BGT)
- ASCII listing file (*modelname*.LST)

The binary files contain head, drawdown and flow exchange values for each grid cell, while the ASCII listing file contains all relevant information on the operation of MODFLOW and the simulation results. The listing (.LST) file is useful if errors occur

during a simulation and you want to know how far MODFLOW progressed or if you want to examine head or drawdown values at given intervals.

For a steady-state simulations, only one set of values for each grid cell are written these files. However, for transient simulations, each grid cell may contain simulation results for each time step, resulting in file that become unnecessarily large. By default the information is saved in the binary files at the end of each stress period and at the end of the simulation for the listing (.LST) file.

The **Output Control** run options set the information and frequency of information written and saved to the various MODFLOW output files (see figure below).



The first two columns list the available stress periods and associated time steps for the entire simulation (only one stress period and time step will be listed for steady-state simulations). The remaining columns indicate the information which can be written and saved to the various MODFLOW output files. To select an output option, click on the appropriate checkbox and a checkmark (✓) will appear to indicate that the selected information will be written for the selected time step.

The columns labelled **Save to Binary** will save the output information to the binary files as described below.

Heads: Saves the heads in the binary heads file (.HDS).

DDown: Saves the drawdown in the binary drawdown file (.DDN).

F.Term: Saves the cell-by-cell flow terms in the binary budget (.BGT) file.[1]

Note: The Zone Budget program uses the .BGT file for calculating the flow between zones. Therefore, to change the frequency at which the Zone Budget information is saved, select the desired **F.Term** intervals.

The columns labelled **Print to LST** will save the output information to the binary files as described below.

Heads: Saves the heads in the listing file.

DDown: Saves the drawdown in the listing file.

F.Term: Saves the flux terms (cell by cell flow terms) in the listing file.

Bud.: Saves the budget information in the listing file.

Note: MODFLOW only allows the flow terms (**F.Term**) to be stored once, in either the binary budget file (.BGT) or the listing file (.LST).

The checkbox labelled ☑ **Save .FLO file**will save the cell-by-cell flow terms required by MT3D when MT3D is not being run.

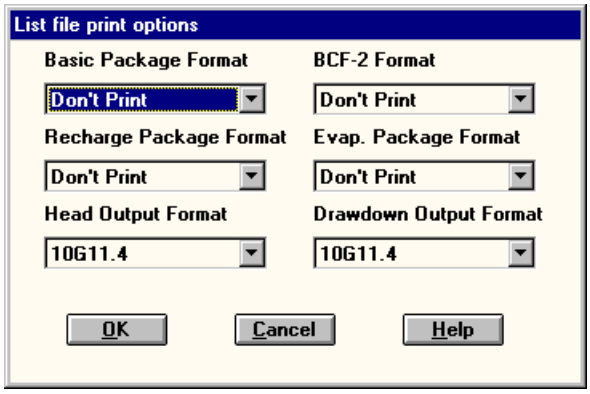
Saving Output Every Nth Time Step

For simulations with many stress periods and time steps it can be very tedious to manually select the desired output time step intervals. The row of fields underneath the Output Control table are used to specify regular time step intervals for saving files during **Each Nth step in each stress period**. The first text box is where the **N** value is entered. To apply this value to the column, click the underlying checkbox.

4.2.9 List File Options

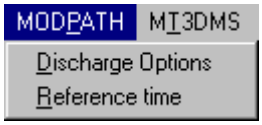
The **List File Print Options** window, as shown below, allows you to specify which information will be written to the listing file (.LST), as well as the format of this information

1. If MODPATH is run with the MODFLOW simulation, Visual MODFLOW will save the flow terms for all time steps



4.3 MODPATH Run Settings

The **MODPATH** program is used for calculating the advective flow pathlines for forward tracking and backward tracking particles. MODPATH has the following run-time settings.



Discharge Options: Select the option to control the discharge of the particles at sinks.

Reference Time: Set the reference time options for particle releases.

4.3.1 Discharge Options

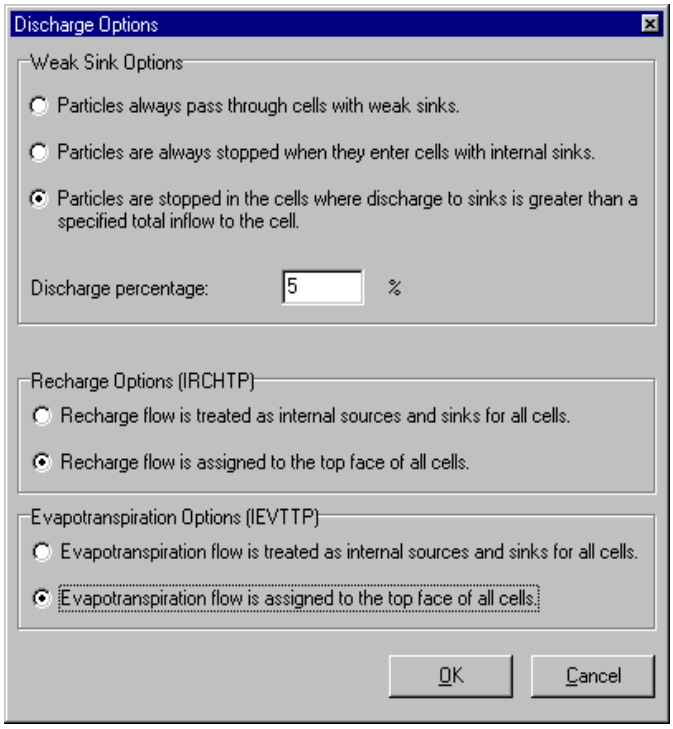
The **Discharge Options** are used to tell MODPATH what to do with particles when they enter a grid cell where water is leaving the system. Any grid cell where water is leaving the system is classified as a "sink". For example, a pumping well is a sink, or all cells in layer 1 with evapotranspiration are sinks.

Weak Sink Options

In many cases the water leaving the system through this grid cells is less than the amount of water entering this grid cell. If this difference is large, the cell is classified as a "weak sink". Since MODPATH cannot always determine if a particle should be removed from the system when it encounters a weak sink, there are three options to control how particles should be treated when sinks are encountered.

- **Particles pass through cells with weak sinks;**
- **Particles are stopped when they enter cells with internal sinks; and**
- **Particles are stopped when discharge to sinks is in excess of a specified percentage of cell inflow. By default this is 5%.**

The desired Weak Sink Option may be selected from the Discharge Options window shown in the following figure.


Discharge Options
Weak Sink Options
Particles always pass through cells with weak sinks.
Particles are always stopped when they enter cells with internal sinks.
Particles are stopped in the cells where discharge to sinks is greater than a specified total inflow to the cell.
Discharge percentage:
5
%
Recharge Options (IRCHTP)
Recharge flow is treated as internal sources and sinks for all cells.
Recharge flow is assigned to the top face of all cells.
Evapotranspiration Options (IEVTTP)
Evapotranspiration flow is treated as internal sources and sinks for all cells.
Evapotranspiration flow is assigned to the top face of all cells.
OK
Cancel

Recharge Options

The **Recharge Options** are used to define how MODPATH treats the Recharge flow entering the system. The **Recharge Options** are:

- **Recharge flow is treated as internal sources and sinks for all cells**
- **Recharge flow is assigned to the top face of all cells**

The first option treats recharge as a distributed source entering the cell from all sides, where the second option treats recharge as though it is entering only through the top face of the cell.

According to MODPATH documentation, the distributed source approximation for areal recharge is usually only appropriate for two-dimensional areal flow models.

Evapotranspiration Options

The **Evapotranspiration Options** are the same as described for Recharge above.

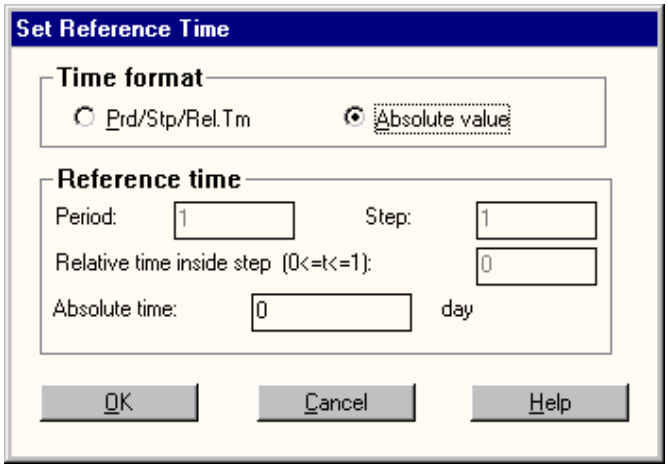
4.3.2 Reference Time Settings

The **Reference Time** is used by MODPATH as the time datum for the simulation of both forward and backward tracking particles. This option is only applicable for transient flow simulations.

The **Release Time(s)** specified for the particles, (see section Particle Release Time on page 151) will be added to the **Reference Time** to determine the actual time of release for each particle.

There are two **Time format** options for setting the **Reference time**:

- **Prd/Stp/Rel.Tm.:** Specify the Reference Time by entering the Stress Period (**Period**), Time Step (**Step**) and **Relative time inside step**.
- **Absolute value:** Specify the reference time as an **Absolute time** from the beginning of the simulation.



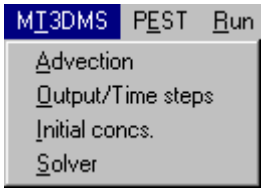
Note: For backward particle tracking in transient simulations, the Reference Time must not be the beginning of the simulation because there are no simulation results before Time = 0.

4.4 MT3D Run Settings

As discussed in Chapter 2, Visual MODFLOW continues to support several different versions of the MT3D contaminant transport modeling program. Depending on which transport numeric engine specified in the model setup, the following names could appear on the top menu bar:

- **MT3D1.5** - Single Species, Public Domain
- **MT3D96** - Single Species, S.S. Papadopulos
- **MT3DMS** - Multi-Species, Public Domain
- **MT3D99** - Multi-Species, S.S. Papadopulos
- **RT3D** - Reactive Multi-Species, Public Domain
- **RT3Dv2.5** - Reactive Multi-Species, Public Domain

Fortunately, each of these different versions of MT3D have similar run settings as described below.



Advection: Select the solution method used to solve the advective terms in the transport equation.

Output/Time Steps: Specify the output times when the transport simulation results will be saved to the output file.

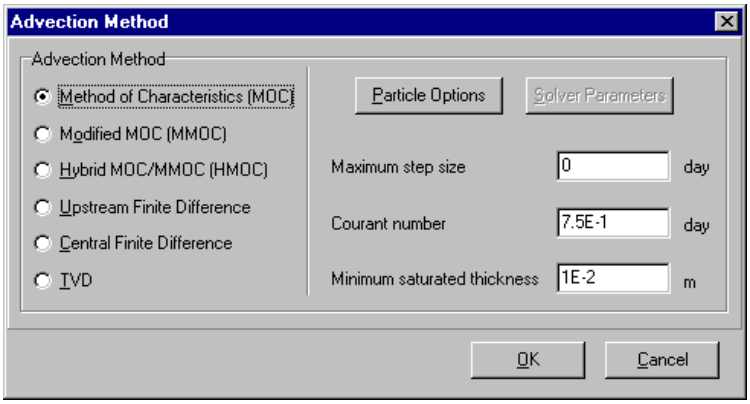
Initial Concs.: Specify the initial concentrations to use.

Solver: Specify the setting for the GCG Solver (available for MT3DMS, MT3D99 and RT3Dv.2.5 only).

4.4.1 Advection Method Settings

The **Advection** settings are used to select the numerical method used to solve the advective part of the transport equation and to customize the settings for the selected method. Modifying the default **Advection** parameters requires some understanding of the techniques used to solve the advection component of mass transport. For additional information, the user is encouraged to refer to the MT3DMS manual. To facilitate reference, the descriptions below retain the symbols used in the MT3DMS manual.

The **Advection Method** dialog for the MT3DMS transport engine is shown in the following figure. Although there are some subtle difference in the Advection settings for different transport engines, the majority of the settings are the same and are described below.



The available **Advection Methods** (MIXELM) are:

- **Method of Characteristics (MOC)**
- **Modified Method of Characteristics (MMOC)**
- **Hybrid Method of Characteristics (HMOC)**
- **Upstream Finite Difference**
- **Central Finite Difference**
- **TVD**

A brief description of these solution methods is provided in the following section.

Unlike the finite-difference method, the mixed Eulerian-Lagrangian schemes (MOC, MMOC, and HMOC) are not entirely based on the principle of mass conservation. Due to the discrete nature of the moving particles, the solution does not guarantee that the mass entering a cell will equal the mass exiting a cell. The resultant mass balance error can be significant at early times, but usually decreases at later times. Various parameters, such as the number and initial distribution pattern of moving particles, the particle tracking scheme, and the step size, can be adjusted to minimize the mass balance discrepancy.

The **Courant Number** represents the number of cells a particle will be allowed to move in any direction in one transport step when the **MOC**, **MMOC** and **HMOC** methods are used. Generally, the **Courant Number** is between 0.5 and 1.0, however values in excess of 1.0 can be used with caution. If the upstream finite difference method is used, the Courant Number must not exceed 1.0. Since the flow terms in all cells in the entire grid are checked when determining the maximum allowable step size for particle tracking, there may be some cells outside the area of interest with high flow rates. The high flow rates in these cells will control the time step calculation in MT3D. In this situation, setting the **Courant Number** greater than 1 will not affect the accuracy of the simulation.

The **Minimum saturated thickness** parameter is used to set a value for the minimum thickness of the saturated layer for each cell. This option is particularly important when

active cells are running dry. This variable will be in the units specified for **Length** during the initial setup of the model.

Advection Methods

The available **Advection Methods** (MIXELM) are described below.

Method of Characteristics (MOC)

The MOC method is available in all versions of MT3D. The MOC method uses a conventional particle tracking technique based on a mixed Eulerian-Lagrangian method for solving the advection term. The dispersion, sink/source mixing and chemical reaction terms are solved with the finite difference method. The MOC technique tracks a large number of moving particles forward in time and keeps track of the concentration and position of each particle.

The main advantage of the MOC technique is that it is virtually free of numerical dispersion. However, the drawback of the MOC technique is that it can be slow and can require a large amount of computer memory.

Modified Method of Characteristics (MMOC)

The MMOC method is available in all versions of MT3D. The MMOC was developed to improve computational efficiency of the MOC technique. Unlike the MOC technique, which tracks the position and concentration of a large number of moving particles, the MMOC technique places a particle at the mid-point of each cell at each new time level. The particle is tracked backward to find its position at the old time level and the concentration associated with the old time level is used to approximate the concentration at the new time level.

The MMOC technique is both faster and requires less computer memory than the MOC technique. However, with the lower-order interpolation scheme available with MT3D the MMOC technique introduces some numerical dispersion.

Hybrid Method of Characteristics (HMOC)

The HMOC method is available in all versions of MT3D. The HMOC technique combines the strengths of the MOC and the MMOC techniques by using an automatic adaptive scheme that uses the MOC technique at sharp concentration fronts and the MMOC technique away from the fronts. By selecting an appropriate criterion for controlling the switch between the MOC and MMOC techniques, the HMOC scheme can provide accurate solutions for both sharp and non-sharp front problems.

Upstream Finite Difference Method

The Upstream Finite Difference method is available in all MT3D versions. Since, the finite-difference method does not involve particle tracking or concentration

interpolations, it is normally more computationally efficient than the Method of Characteristics (MOC). In addition, the finite difference method normally has very small mass balance errors because it is based on the principle of mass conservation. However, the Upstream Finite-Difference method can lead to significant numerical dispersion for problems having sharp concentration fronts.

Central Finite Difference Method

The Central Finite Difference method is only available in MT3DMS, MT3D99 and RT3Dv.2.5. The central finite difference method does not exhibit the numerical dispersion problems like the Upstream Finite Difference method, but is susceptible to excessive artificial oscillations in advection dominated problems.

TVD Method

The TVD method is available only with MT3DMS, MT3D99 and RT3Dv.2.5. The third-order total-variation-diminishing (TVD) scheme, which is mass conservative, solves the advection term based on ULTIMATE algorithm (Universal Limiter for Transient Interpolation Modeling of the Advective Transport Equations). As in the particle-based methods, the TVD scheme solves the advection component independent of the other terms in the transport equation.

Results from the third-order TVD scheme may exhibit minor numerical dispersion and minor oscillations in problems having sharp concentration fronts. Since the algorithm is explicit there is a stability constraint on the step size. The maximum allowed value for the time step is the minimum time step calculated for every active cell.

Technical Note on the Generalized Conjugate Gradient Solver

A new implicit Generalized Conjugate Gradient (GCG) solver is available for MT3DMS, MT3D99 and RT3Dv2.5. This solver is general-purpose iterative solver based on the generalized conjugate gradient method and is implemented in a new package called the Generalized Conjugate Gradient (GCG) Package. The GCG solver is usually faster than the explicit finite-difference method because there is no time step constraints. However, it requires significantly more memory than the explicit solution method.

The explicit method, on the other hand, is simple and requires much less memory than the implicit method. It is also computationally efficient for certain advection-dominated problems in which the transport step size is not limited by stability constraints but rather by accuracy considerations. However, for transport problems with fine grid spacing, large dispersion coefficients, strongly non-linear sorption, or strong sink/source terms, the stability constraints can lead to exceedingly small transport steps when the explicit method is used.

The following is a technical note provided by Mr. Christopher J. Neville of S.S. Papadopulos & Associates describing how the GCG Solver is implemented.

General Methodologies of the Solution Methods

I. When the particle-based methods (MOC, MMOC and HMOC) and the TVD method are used to simulate solute transport, the governing equation is split into two parts. On the left-hand side are the mass accumulation term and the advection term (in the fluid mechanics literature, the sum of these two has been referred to as the total derivative of the concentration with respect to time, Dc/Dt). On the right-hand side, the dispersion, reactions, and source-sink mixing terms are represented with finite-difference approximations.

II. When the "pure" finite difference methods are used (FD), all terms in the governing equation are treated simultaneously, with advection, dispersion, reactions, and source-sink mixing terms represented with finite-difference approximations.

Treatment of the transport terms with respect to time

MT3D now offers the user two options for evaluating the terms in the finite-difference approximations, explicit or implicit-in-time weighting.

I. For explicit-in-time, or forward-in-time weighting (FIT), the terms in the finite-difference approximations are evaluated at the previous time step. This was the only option available in versions of MT3D from v.1.1 to MT3D96. Explicit-in-time weighting has the advantage of not requiring the assembly, storage, and solution of a matrix. It requires the least amount of RAM of all feasible methods. In particular, it requires no additional RAM with respect to the corresponding MODFLOW model. This was an important requirement for the development of MT3D, since the code was developed on a PC, for implementation on PCs. We now live in a world in which RAM is inexpensive. However, when MT3D was developed in 1987-1988, additional RAM over 640 KB was very limited and very expensive. Explicit-in-time weighting has the disadvantage of not being stable unless tight restrictions on the size of time steps are satisfied. In many cases, the size of the time steps could be very small - and would only get smaller as the spatial resolution of a model was increased. Furthermore, in versions of MT3D preceding MT3D96, the calculation of the overall maximum allowable step size was not correct, and model could still experience severe problems although it seemed that all stability criteria were being satisfied. In theory, the maximum Courant number may be 1.0. However, because the stability requirements were not calculated correctly, in practice we had to specify maximum Courant numbers significantly smaller than 1.0 to ensure stability (often as low as 0.1).

II. For implicit-in-time, or backward-in-time weighting (BIT), the terms in the finite-difference approximations are evaluated at the current time step. This option was added with the introduction of MT3DMS and MT3D99. Implicit-in-time weighting has the advantage of being unconditional stable, and allows the use of relatively large time steps. The option requires the assembly, storage,

and solution of a matrix, but these requirements are not as onerous as they were, both because additional RAM is relatively inexpensive, and because accurate and efficient matrix solvers are now widely available. The disadvantage of the method is that it is now possible to create transport models that require much more storage than the corresponding MODFLOW model. Although implicit-in-time weighting is unconditionally stable, its accuracy is not assured if the time steps are too large. In order to guarantee the accuracy, the maximum Courant number may be limited to 1.0. As a simulation proceeds and the concentration gradients diminish, this requirement may be relaxed.

Time-weighting options with the particular MT3D solution methods

I. When the particle-based methods (MOC, MMOC and HMOC) and the TVD method are used to simulate solute transport, the terms on the right-hand side (the dispersion, reactions, and source-sink mixing) may be represented with either explicit or implicit-in-time weighted finite-difference approximations.

II. When the "pure" finite difference methods are used (FD), all terms in the governing equation may be represented with either explicit or implicit-in-time weighted finite-difference approximations.

Using the GCG Solver

When the GCG Solver Package is specified to be included in a simulation, MT3D will do the following:

I. When the particle-based methods (MOC, MMOC and HMOC) and the TVD method are used to simulate solute transport, the terms on the right-hand side are represented with implicit-in-time weighted finite-difference approximations.

   At the risk of confusing the issue, I should add at this point that the TVD algorithm implemented in MT3D is explicit-in-time. This means that even if the GCG Package is used, the times steps in TVD run will be still be subject to a time constraint - but only the advection term.

II. When the "pure" finite difference methods are used (FD), all terms in the governing equation are be represented with implicit-in-time weighted finite-difference approximations.

   If the user does not specify the use of the GCG package, then all terms are represented with explicit-in-time weighted finite-difference approximations.

Particle Options

The **[Particle Options]** button is only available when one of the particle-based **Advection** methods is selected for solving the advection part of the transport equation.

The **[Particle Options]** button opens the **Particle Parameters** dialog as described below.

There are three different **Particle Tracking Methods** available:

- **First-order Euler algorithm,**
- **Fourth-order Runge-Kutta algorithm, and**
- **Fourth-order Runge-Kutta for sinks and sources, Euler elsewhere**

Traditionally, the **First-order Euler algorithm** is used for particle tracking. A uniform step size is used for all moving particles during each transport step in the particle tracking calculations. For particles located in areas of relatively uniform velocity, the **First-order Euler algorithm** may be sufficiently accurate. However, for particles in areas of strongly converging or diverging flows (for example, near sources or sinks), a higher order algorithm such as the **Fourth order Runge-Kutta algorithm** may provide a more accurate solution. Although the **Fourth-order Runge-Kutta algorithm** is more accurate and permits the use of larger tracking steps, the computational requirements are high for problems with a large number of particles.

The **Particle Parameters** associated with the various **Particle Tracking Methods** are described below.

- **Conc. Weighting Factor (WD)** is a fraction between 0 and 1, and is normally 0.5. The higher/lower the factor, the higher/lower the concentration for the particles within a cell. Generally, it can be increased toward 1.0 as advection dominates. Adjusting this number can sometimes improve the mass balance.
- **Max. Number of Particles (MXPART)** is the maximum number of total moving particles allowed in the domain. It is only used for the MOC and HMOC techniques.
- **Min Particles/Cell (NPMIN)** is the minimum number of moving particles allowed per cell. If the number of particles in a cell at the end of a transport step is less than NPMIN, new particles are inserted into that cell to maintain a sufficient number of particles. NPMIN can be set to 0 in relatively uniform flow fields, and a number greater than zero in diverging/converging flow fields. Generally, NPMIN is between 0 and 4.
- **Max Particles/Cell (NPMAX)** is the maximum number of moving particles allowed per cell. If the number of particles exceeds NPMAX, particles are removed from that cell until NPMAX is met. Generally, NPMAX can be set to a value approximately twice the value of NPH (described below).
- **Number of Planes (NPLANE)** is the number of horizontal planes on which initial particles are placed within each cell block must be specified. For two-dimensional simulations or plan view, choose a single horizontal plane. For cross-sectional or three-dimensional simulations, two horizontal planes are normally adequate. Additional horizontal planes may be added if more resolution in the vertical direction is required.
- **Negligible Gradient (DCEPS):** is used to improve the computational efficiency of the MOC procedure. A higher number of particles are placed in

cells involving advection calculations and a lower number of particles are placed in cells not involved in advection calculations. If the calculated relative concentration gradient between adjacent cells is greater than DCEPS, NPMAX particles are placed in the cell. If the calculated relative concentration gradient is less than DCEPS, NPMIN particles are placed in the cell. A very small value such as 10^{-5} is generally used.

- **Number of Particles for C <= Negligible Gradient (NPL)** is the number of initial particles per cell to be placed at cells where the calculated concentration gradient is less than or equal to DCEPS. Generally, this number can be set to 0. Setting NPL equal to NPH causes a uniform number of particles to be placed in every cell over the entire grid.
- **Number of Particles for C > Negligible Gradient (NPH)** is the number of initial particles to be placed at cells where the concentration gradient in the cell (DCCELL) is greater than DCEPS. In relatively uniform flow fields use a smaller NPH and increase NPH as the non-uniformity of the flow field increases. Values exceeding 16 in two-dimensional flow or 32 in three-dimensional flow are rarely necessary.
- **Critical Conc. Gradient (DCHMOC:** is the relative concentration gradient between the cell being considered and its neighbouring cells and is used to evaluate the sharpness of the concentration front. If the HMOC scheme is being used and the calculated relative concentration gradient is greater than DCHMOC then the MOC scheme is used, otherwise the MMOC scheme will be used. The DCHMOC criterion is empirical, but values between 0.001 and 0.01 have been found to be generally adequate for most problems.
- **Particle Pattern (NLSINK)** sets the number of particles per horizontal plane. The fixed pattern option distributes a fixed number of particles over the cell in the pattern shown in the pattern box. The total number of particles in the cell is multiplied by NPLANE. This option works well for relatively uniform flow fields.

The random pattern option distributes the particles randomly in both the horizontal and vertical directions. The number of particles is entered under NPH (described below). If the flow field is non-uniform, this option may capture the essence of the flow field better than the fixed pattern. The random distribution also leads to smaller mass balance discrepancy in non-uniform or diverging/converging flow fields.

Solver Parameters

The **[Solver Parameters]** button is active when you select either the **Upstream Finite Difference Method** or the **Central Finite Difference Method**. These are the only two methods that can use the implicit GCG solver when calculating the advective component of the advection-dispersion equation. The other components of the transport equation (Dispersion, Decay, etc) are always solved using the finite-difference method. The implicit solver can be used to solve this part of the equation for the particle-based

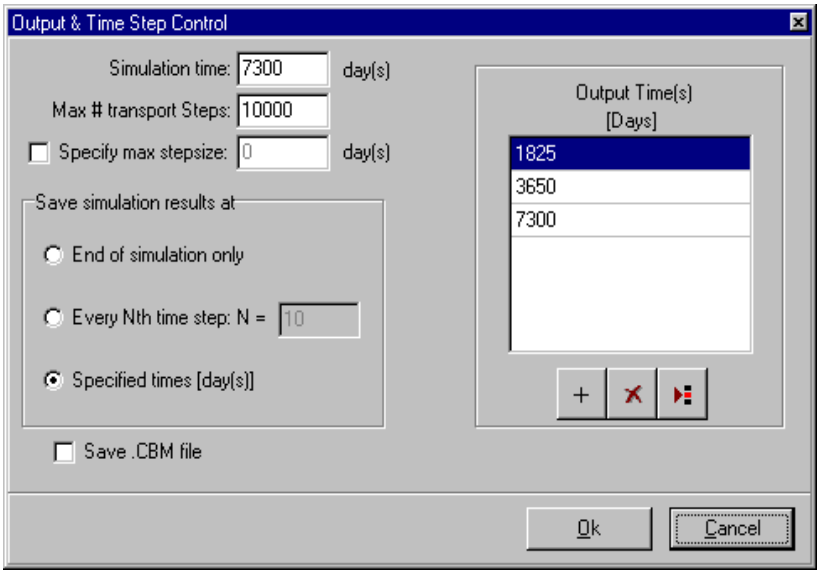
methods and the TVD method. However, in this case the solver must be set up by selecting **MT3D/Solver** from the top menu bar of the **Run** section.

In MT3D1.5, MT3D96 and RT3Dv1.0, the GCG Solver is not available and the finite difference method will always be solved explicitly.

Advection Method	Advantages	Disadvantages	Appropriate Conditions
Implicit Finite Difference (with implicit GCG solver)	Computationally efficient Minimal mass balance errors Faster than the explicit method	Numerical dispersion	Dispersed fronts Peclet <2
Explicit Finite Difference (without implicit GCG solver)	Computationally efficient Minimal mass balance errors	Numerical dispersion	Dispersed fronts Peclet <2
Method of Characteristics	Low numerical dispersion	Not mass conservative Potential for mass balance errors	Non-dispersed fronts Peclet >10
Modified Method of Characteristics	Computationally efficient	Numerical dispersion Not mass conservative Potential for mass balance errors	Dispersed fronts Peclet <0.1
Hybrid Method of Characteristics	Computationally efficient Low numerical dispersion	Must select adaptive criterion Not mass conservative Potential for mass balance errors	All conditions

4.4.2 Output/Time Steps Settings

The **Output/Time Steps** settings are used to define the length of the transport simulation and the times at which the results will be saved to the binary concentration file (.UCN). The **Output & Time Step Control** dialog window is shown in the following figure, while the individual settings are described below.



- **Simulation time:** is the total length of the transport simulation in the specified time units. This must be greater than zero.
- **Max # of transport steps:** is the maximum number of transport steps for the simulation. Once the simulation has run through the specified Max # of transport steps the model will stop. This parameter is primarily used to limit the size of the output files generated.
- **Specify max stepsize (DT0)** is the maximum step size to use for each transport time step. MT3D will use the smaller of either the internally calculated maximum timestep size based on the courant number, or the maximum timestep size specified here. If the implicit GCG solver is used, this value is ignored and the value found in the Solver options is used instead.
- **Save simulation results at End of simulation only** will save the simulation results at the end of the simulation only and will not save any intermediate results. If this option is not selected the solute concentrations can be save at either regular time step intervals (**Every Nth time step**) or at manually entered times (**Specified times**).

Calculating Transport Timestep Sizes (Particle-Based Methods)

MT3D calculates the transport timestep size for the particle-based methods (MOC, MMOC, HMOC) and the explicit finite-difference methods. The explicit finite difference methods and the particle-based methods use a uniform timestep size for all transport timesteps, which is calculated based on the following three numerical criteria.

The Courant Condition:

$$|\Delta t| \leq \gamma_c R_{min} \left(\frac{\Delta x}{v_x}, \frac{\Delta y}{v_y}, \frac{\Delta z}{v_z} \right)$$ (Eq. 4.8, MT3D Reference Manual)

Numerical Stability for Dispersion:

$$\Delta t \leq \frac{0.5R}{\left(\frac{D_{xx}}{\Delta x^2} + \frac{D_{yy}}{\Delta y^2} + \frac{D_{zz}}{\Delta z^2} \right)}$$ (Eq. 4.28, MT3D Reference Manual)

Numerical Stability for Source and Sink Terms:

$$\Delta t \leq \left| \frac{R^n_{i,j,k} \vartheta_{i,j,k}}{q^n_{s\,i,j,k}} \right|$$ (Eq. 4.32, MT3D Reference Manual)

The minimum value for the entire active model is used. This timestep size cannot be increased and unfortunately, can lead to excessively small time steps in many situations.

From the three criteria above, it is evident that when cells are small, or velocities are large, the minimum time step may be small. Therefore, the first thing to be done to control the calculated transport step size is to make all cells outside the area of interest, that could control the step size, inactive for transport. For example, the area around pumping wells outside the zone of interest could be made inactive for transport.

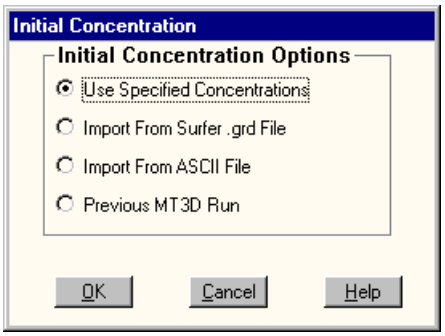
The MT3D output file (***.OT**), contains a useful summary of the three calculated time step criteria. The summary includes the co-ordinates (row, column, layer) of the three cells controlling the transport time step. Depending on the saving frequency of simulation results, this file can be quite large; therefore load it into a text editor and search on 'STEPSIZE' to find the criteria. However, if the simulation has been interrupted, then these lines may not be printed. Finally, if the simulation time is still excessive, the best tactic may be to find a faster computer for running the MT3D simulations.

However, the best advice may be to switch to the implicit finite-difference method.

For more information on the way that MT3D calculates the transport time step, please see the MT3D Reference Manual. Descriptions of the criteria can be found in Chapter 4, pages 4-5, 4-19 and 4-20.

4.4.3 Initial Concentrations Settings

The **Initial Concentrations** settings are used to specify the source of the initial concentration data (see the following figure).



If the model is simulating contaminant migration immediately following a contamination event, then the initial concentrations of all contaminant species will likely be zero. However, if the model is simulating reactive transport of contaminants, the initial concentrations of species such as dissolved oxygen (O2), sulphate (SO4), nitrate (NO3) and ferrous iron (Fe3) will need to be set equal to measured (or estimated) background concentrations.

As with the **Initial Heads** run settings, there are four option for defining the initial concentration value of the model.

- **Use Specified Concentrations** will use the initial concentrations specified in the **Input** section of Visual MODFLOW. If no initial concentrations were specified for a given solute, Visual MODFLOW will automatically set all initial concentrations equal to zero.
- **Import from Surfer .grd File** will use data from selected Surfer file(s) to calculate the initial concentrations of each species for each layer of the model. See the section Importing Initial Concentrations below.
- **Import from ASCII File** will use data from selected ASCII file(s) to calculate the initial concentrations of each species for each layer of the model. See the section Importing Initial Concentrations below.
- **Previous MT3D Run** will use the binary format concentrations file (.UCN) from a previous MT3D model simulation as the initial concentrations for the current simulation. The selected .UCN file must have the same number of rows, columns and layers as the current model and it must have the same number of species.

Importing Initial Concentrations

Visual MODFLOW can import initial concentration data from either **ASCII** files (.TXT) or **Surfer** files (.GRD) in world or model co-ordinate systems.

The ASCII files must be comma or tab delimited with the following format:

X-Coord., Y-Coord, Concentration Value

For example:

1120, 2352, 0.023

3392, 4491, 0.008

2892, 2531, 1.500

3590, 1803, 0.532

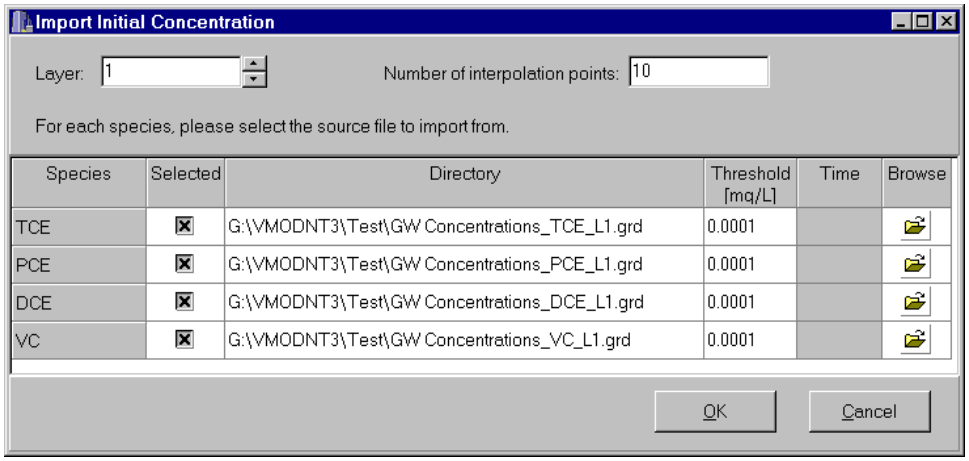
No header information or column titles are allowed and the coordinate locations for the data points must be within the model domain. If different initial concentration values are required for different sets of layers in the model, then separate ASCII text files must be prepared for each set of model layers.

The Surfer Grid files must be saved in binary format and the majority of the grid domain must correspond with the model domain. If different initial head values are required for different sets of layers in the model, then separate Surfer Grid files must be prepared for each set of model layers

Visual MODFLOW uses an inverse distance interpolation method to calculate the initial concentration value for the center of each grid cell.

The following steps can be following to import initial concentrations from an **ASCII** file or a **Surfer** file.

- Choose the source file type from the **Initial Concentrations** dialog and then click the **[OK]** button.
- An **Import Initial Head** dialog will appear for Layer 1 as shown in the following figure.
- Click the checkbox in the **Selected** column to indicate the contaminant species which will use initial concentration values imported from a file.
- Click the **[Browse]** icon to select the initial concentration source file for each contaminant species.
- To use different initial concentration source files for different model layers, click the **[Up]** or **[Down]** arrow buttons next to the **Layer** field.
- Click **[OK]** to interpolate the initial heads data to the model grid and import the array into Visual MODFLOW.

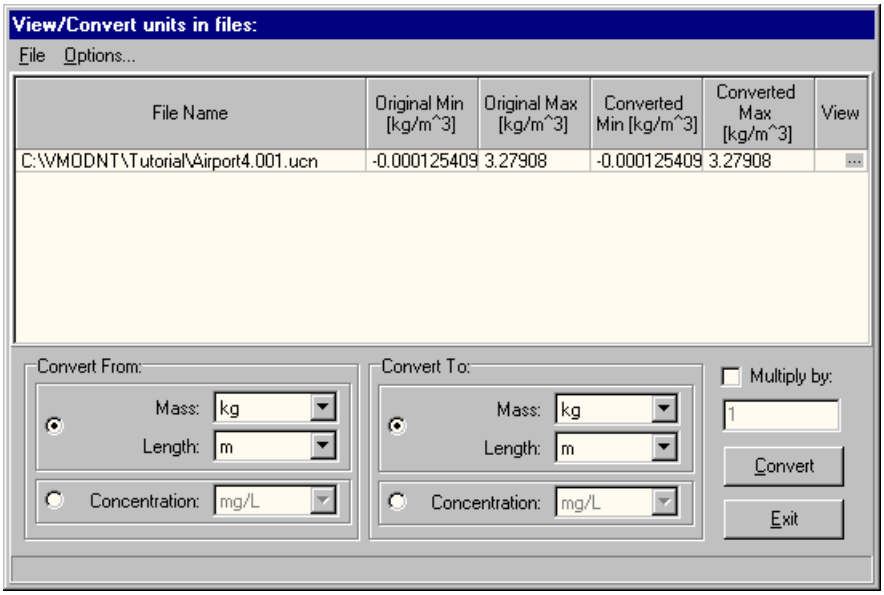


The **Threshold** value for each species is the lowest initial concentration value assigned to any grid cell in the specified layer. Any initial concentration values less than the **Threshold** value will be assigned a value of zero.

The **Number of interpolation points** is the maximum number of nearest data points Visual MODFLOW will use to interpolate the initial concentration data to the model grid.

4.4.4 UCN Conversion and Creation Utility

This feature allows the user to convert concentration files to appropriate consistent mass and length units. If you select the **View/Convert Initial Concs.** option, the following window appears:



To view or convert a file select **File/Open** from the top menu bar and choose the .UCN file to convert.

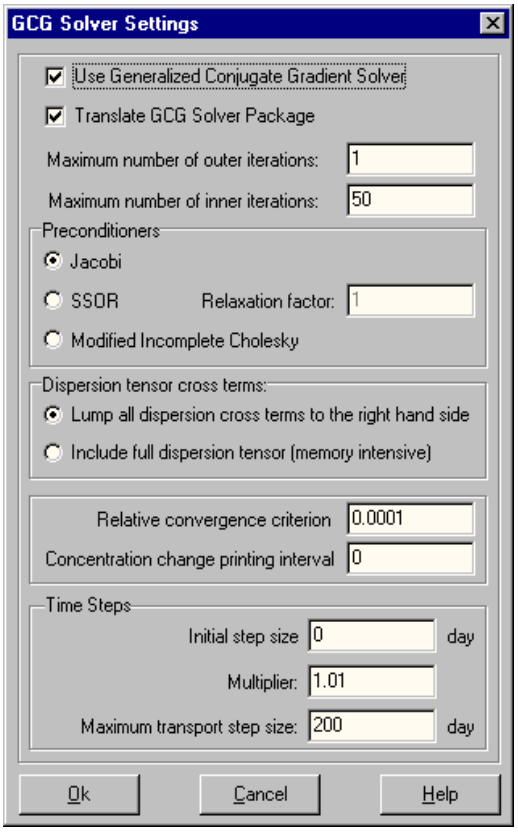
The **Options...** menu item provides the option to convert files either by updating the files in place (default option) or creating the files with added extension ".new".

The selected file path to be edited will appear under the heading **File Name**. The **Minimum** and **Maximum** concentration values allows the user to identify appropriate values and units. The converted concentration values will update as units are selected in the **Convert From** and **Convert To** fields. The **View [...]** button loads the **VM Viewer** window displaying a contour map of the concentrations.

Once the desired settings are achieved, press the **[Convert]** button to convert the selected file(s).

4.4.5 Solver Settings

The **Solver** run settings control the operation of the Generalized Conjugate Gradient (GCG) Solver. This option is available only for transport variants using the MT3DMS or MT3D99 numeric engines. The **GCG Solver Settings** dialog window is shown in the following figure as described below.



For details concerning the implicit GCG Solver and its parameters, please refer to the MT3DMS manual. For ease of reference, the variable names, used within the MT3DMS manual, are in brackets beside each parameter.

- **☑ Use Generalized Conjugate Gradient Solver** indicates whether the GCG Solver will be used to solve the non-advective terms in the transport equation.

  If one of the finite-difference methods is selected for the **Advection Method** then all of the terms in the advection-dispersion equation will be solved implicitly.

  If one of the particle-based methods (MOC, MMOC, HMOC) is selected for the **Advection Method** then only the advection part of the advection-dispersion equation will be solved implicitly.

- **☑ Translate GCG Solver Package** indicates the GCG solver package will be translated and the GCG package file (*projectname*.*GCG*) will be created. If this option is not selected, the GCG package file will not be created by Visual MODFLOW, but the GCG solver can still be run with MT3DMS if a GCG package file (projectname.GCG) is copied to the working directory of the model.
- **Maximum number of outer iterations (MXITER)**: [Default = 1] The outer loop in the iteration process updates all the coefficients that are concentration-dependent. The default number of outer iterations is one. It should be set to an integer greater than one only when a non-linear sorption isotherm is included in simulation. For further detail please refer to page 4-19 in the MT3DMS Documentation and User's Guide.

- **Maximum number of inner iterations (ITER1)**: [Default = 50] The inner loop in the iteration process continues to iterate toward the solution until the convergence criterion is obtained or the maximum number of inner iterations is reached. During these iterations, the coefficient matrix and the right hand side vector matrix remain unchanged. The default number of inner iterations is fifty. A maximum value of thirty to fifty inner iterations should be sufficient for most problems. For further detail please refer to page 4.19 in the MT3D MS Documentation and User's Guide.

Preconditioning Methods

The GCG Solver implicitly solves the non-advective terms in the transport equation using a two iteration loop process and the choice between three pre-conditioning options:

- **Jacobi** (ISOLVE=1)
- **SSOR (**ISOLVE=2)
- **Modified Incomplete Cholesky (**ISOLVE=3)

The **Modified Incomplete Cholesky** method usually converges faster than the other two method options, but it requires significantly more memory.

Dispersion Tensor Cross Terms

The GCG Solver has two options for dealing the cross-derivative terms of the dispersion tensor:

- **Lump all dispersion cross terms to the right hand side (NCRS=0)** will place all the dispersion tensor cross terms to the right hand side of the matrix equation and consider them as know values. This method approximates the equation (the loss of accuracy is generally insignificant) but is highly efficient (reduces the memory requirement by nearly two thirds) since there are significantly less unknown terms to be solved. For further detail please refer to the MT3D MS Documentation and User's Guide.
- **Include full dispersion tensor (NCRS=1)** will keep all the dispersion tensor cross terms on the left-hand side of the matrix equation and consider them as unknown terms. This method gives the exact matrix equation but is memory intensive since there are significantly more unknown terms to be solved. For details refer to the MT3D MS Documentation and User's Guide.

The **Relative convergence criterion (CCLOSE)** [Default = $1x10^{-4}$] is used to judge the convergence, in terms of relative concentration, of the inner iterations of the solver. The default value is 10^{-4}. A value between 10^{-4} and 10^{-6} is generally adequate.

The **Concentration change printing interval (IPRGCG)** [Default = 0] is the interval for printing the maximum concentration changes of each iteration. The default is 0 for printing at the end of each stress period.

Time Steps

- **Initial Step Size (DT0)**: [Default = 0] The **Initial Step Size** is used to override the automatically calculated initial time step. The user can assign a value to be used for the first iteration of the solution. The default value of 0 means that the MT3D calculated value will be used.

  If one of the particle-based methods is used, the maximum timestep size calculated by MT3D will be used unless this value is smaller.

  If the implicit solver is not selected, then this value will be ignored and the value for DT0 will be taken from the **Output/Time Step Control** dialogue.

- **Multiplier (TTSMULT)** [Default = 1] This is the multiplier used to calculated the size of the next transport time step when the finite difference method is used with the implicit GCG solver. A value between 1 and 2 is generally adequate. Using a time step multiplier will degrade the solution at later times when the timestep becomes large, but can significantly decrease the amount of time needed for the solution. If one of the particle-based methods or the TVD method is used, this value will be ignored.
- **Maximum transport step size (TTSMAX)**: [Default = 0] This value is the maximum time step size allowed when a multiplier greater than 1 is used. Setting this equal to zero (default) imposes no maximum limit.

4.5 PEST Run Settings

PEST is an acronym for Parameter ESTimation. For groundwater modeling applications, PEST is widely considered the most powerful and robust parameter estimation program available for automating and improving the model calibration. The way PEST works is by optimizing a set of user-defined model parameters in order to minimize the calibration residuals from a set of user-defined observations. A detailed description of parameter estimation technology and the PEST program is provided in the PEST User's Manual provided with the Visual MODFLOW installation CD-ROM.

Typically, PEST is used to guide the model calibration process towards the most reasonable set of parameter values which result in a good calibration. As a result, it is highly recommended that PEST be used only after the model has been run several times using initial estimates for the model parameters to validate the conceptual model. Once the model is able to converge to a reasonable solution, then PEST can be used to optimize selected model parameters in order to achieve a better calibration result.

It is important to be aware that the "optimized" parameter values calculated by PEST may not be the only combination of parameter values capable of achieving this calibration result, and in fact, the calculated parameter values may not even be 'reasonable' estimates for these parameters. PEST does not differentiate between a sand and gravel aquifer or a clay confining unit, it simply uses the information it has to estimate a combination of parameter values that minimized the objective function.

Visual MODFLOW is seamlessly integrated with WinPEST, a 32-Bit native Windows version of the PEST program. This is a fully functional version of PEST and is not limited by the model size or number of grid cells.

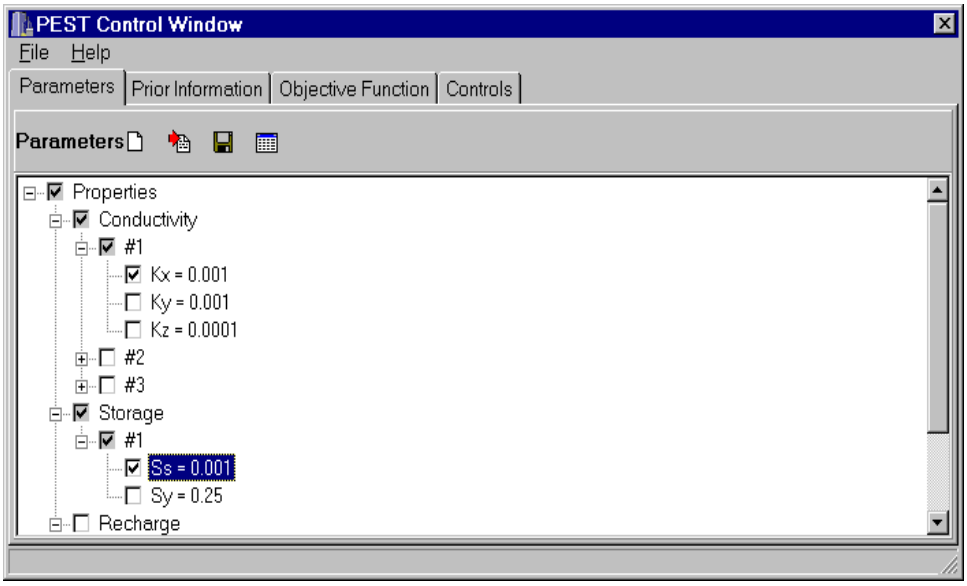
The **PEST** run settings are used to:

- Select the **Parameters** to optimize and specify the parameter settings
- Define **Prior Information**
- Define the **Object Function** settings (observations)
- Set the PEST **Control** Parameters

The steps required to prepare a PEST simulation are described below.

4.5.1 Selecting the Parameters to Optimize

The **PEST Control Window** opens to the **Parameters** selection tree view as shown in the following figure.

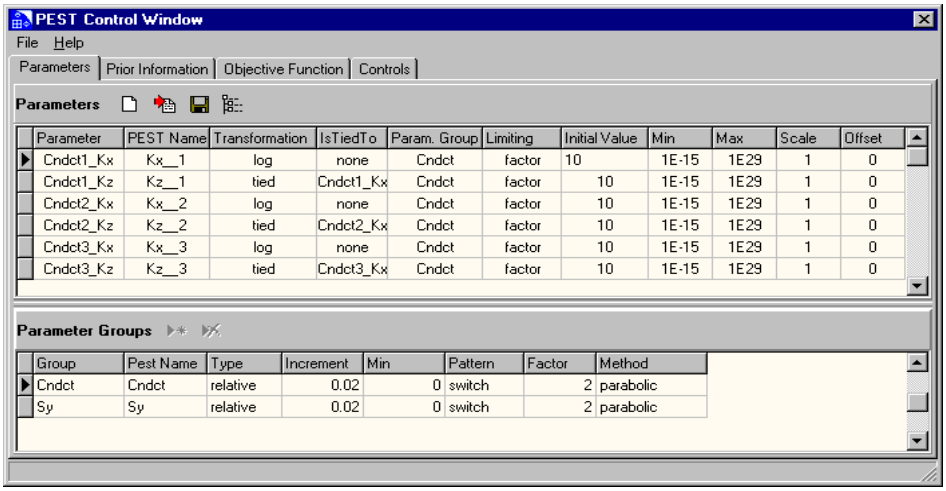


This tree view includes the model parameters which are available for optimization using WinPEST. To expand each branch of the tree simply click the [+] next to each branch. The current version of Visual MODFLOW supports the optimization of the model flow **Properties** including **Conductivity**, **Storage** and **Recharge** parameters. This list of available parameters will be extended in future versions to include virtually all Visual MODFLOW parameters for both flow and contaminant transport simulations.

Individual parameters from each property zone may be easily selected by clicking the [+] icon to expand the branches and then clicking the checkbox next to each parameter.

It is not recommended to select more than 10 parameters to optimize because it significantly increases the simulation time required and may impede the actual optimization process.

Once the parameters have been selected in the **Parameters** tree view, click on the **Table** icon in the menu bar to switch to the **Parameters** table view as shown in the following figure.


PEST Control Window
File Help
Parameters Prior Information Objective Function Controls
Parameters
Parameter PEST Name Transformation IsTiedTo Param. Group Limiting Initial Value Min Max Scale Offset
Cndct1_Kx Kx__1 log none Cndct factor 10 1E-15 1E29 1 0
Cndct1_Kz Kz__1 tied Cndct1_Kx Cndct factor 10 1E-15 1E29 1 0
Cndct2_Kx Kx__2 log none Cndct factor 10 1E-15 1E29 1 0
Cndct2_Kz Kz__2 tied Cndct2_Kx Cndct factor 10 1E-15 1E29 1 0
Cndct3_Kx Kx__3 log none Cndct factor 10 1E-15 1E29 1 0
Cndct3_Kz Kz__3 tied Cndct3_Kx Cndct factor 10 1E-15 1E29 1 0
Parameter Groups
Group Pest Name Type Increment Min Pattern Factor Method
Cndct Cndct relative 0.02 0 switch 2 parabolic
Sy Sy relative 0.02 0 switch 2 parabolic

The Parameters table view is used to define the **Parameter** settings and **Parameter Groups** settings. Each of these settings and the options available for each setting are described in detail in the PEST Reference Manual and in Chapter 4 of the WinPEST User's Manual. The **Parameter Groups** table lists the different groups that PEST will assign the Visual MODFLOW parameters to. The Parameter Groups are used for grouping parameters whose derivatives share common characteristics.

4.5.2 Defining Prior Information

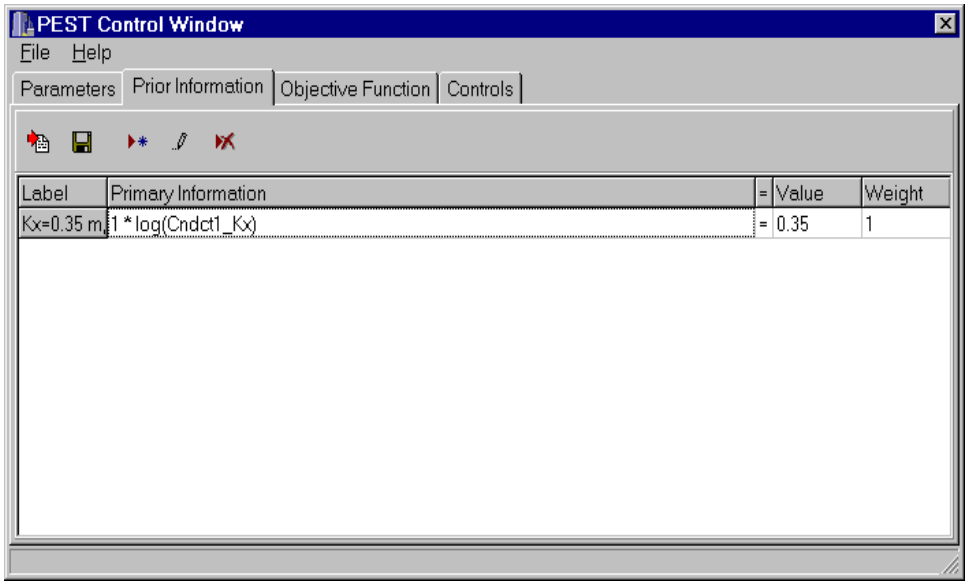
Prior Information is used to define some independent information that exists about the selected parameters. This information may be in the form of unrelated estimates of parameter values, or of relationships between parameters. When this information is included, it can lend stability to the parameter estimation process, especially when parameters are highly correlated. Correlated parameters can lead to non-unique parameter estimates because varying them in certain linear combinations may cause very little change in the objective function. In some cases, this non-uniqueness can even lead to numerical instability and failure of the estimation process. However if something is known about at least one of the members of such a troublesome parameter group, this information, if included in the estimation process, may remove the non-uniqueness and provide stability.

For a detailed description of how Prior Information is incorporated into the PEST algorithm, see Chapter 2 of the WinPEST User's Manual.

Prior Information must be of a suitable type to be included. Both simple equality and linear relationships are acceptable. A weight must be included with each article of prior information. In theory, this weight should be inversely proportional to the standard deviation of the right hand side of the prior information equation. In practice, however, the user simply assigns the weights according to the extent to which he/she wishes each article of Prior Information to influence the parameter estimation process.

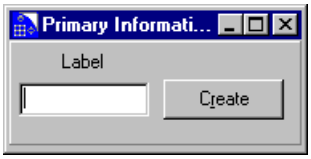
The **Prior Information** tab is shown in the following figure. The steps required to prepare Prior Information articles is described below

.



To add a Prior Information article,

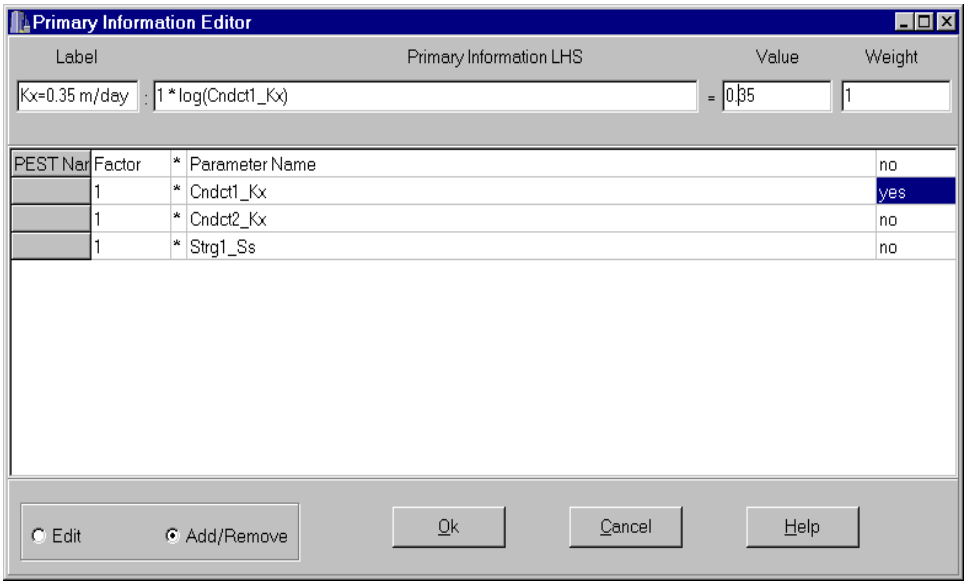
- Click the **Add New Prior Information Article** icon in the toolbar,
- Enter a **Label** (name) for the Prior Information article and then press the **[Create]** button
- A **Primary Information Editor** dialog will appear as shown in the following figure



The **Primary Information Editor** dialog is used to construct the equations defining the new Prior Information article. If no parameters appear under the **Parameter Name** heading, close this dialog and press the **[Save]** icon in the **PEST Control Window** to register the selected parameters.

The field at the top of the dialog labelled **Primary Information LHS** is where the left hand side of the Prior Information equation is defined. Any or all of the available

parameters listed under the **Parameter Name** column can be added to the equation by changing the field under the **Chosen** column from **No** to **Yes** as shown in the following figure.



Note: If the selected parameter is being log transformed by PEST, then the parameter must also be log transformed in the Prior Information article.

In the figure above, the **Primary Information** equation indicates that log of the Kx value from Zone 1 [**1*log(Cndct1_Kx)**] should have a value of 0.35.

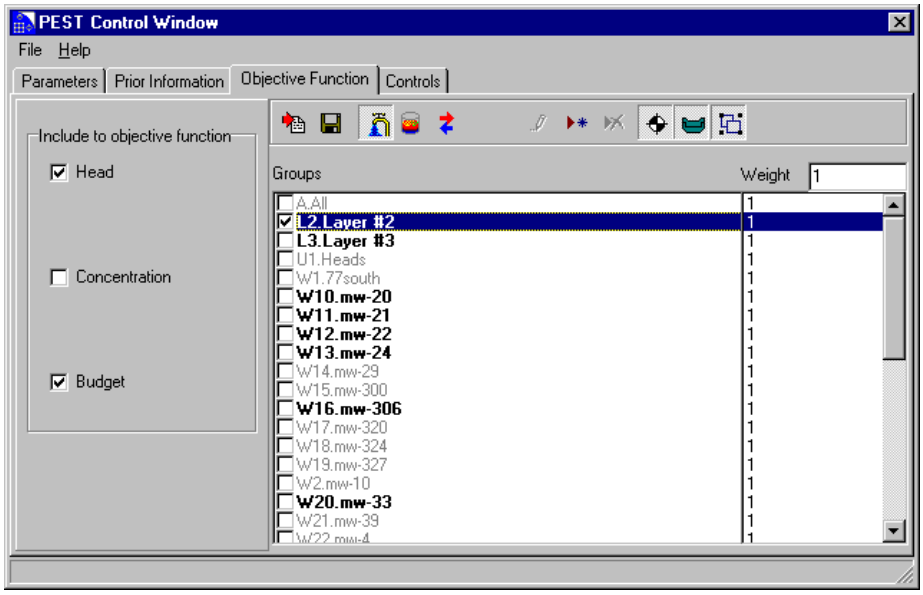
PEST will try to find the set of parameters that minimizes the objective function, while trying to keep this value as close to 0.35 as possible. The higher the weight, the greater will be the impact on the objective function.

The **Factor** column is used to adjust the multiplier for each parameter in the **Primary Information** equation. For example, a negative value may be needed to establish equality between two different parameters such as:

1*log(Cndct1_Kx) * -1*log(Cndct2_Kx) = 0

4.5.3 Defining the Objective Function

The Objective Function defines the data which must be matched by the calculated results in order to calibrate the model. The **Objective Function** tab shown in the following figure is used to select the observations which will be used to calculate the objective function. Selecting the **Objective Function** tab display a list of all available head, concentration or flow observations.



The **Include to objective function** section of the dialog is used to select which data types (**Head**, **Concentration** and/or flow **Budget**) will be used to calculate the objective function.

The **Groups** list contains a listing of the available observation groups which may be used to calculate the Objective Function.

The **Weight** field is used to assign a weight to selected observation **Groups**. The weight is used for two purposes:

- To give more 'importance' to selected observations, or
- To 'normalize' the observation values for different data types

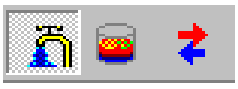
To assign a weight to a selected observation group, click on the **Group** name and then type the desired weight in the **Weight** field and press the <**Enter**> key.

The toolbar located at the top of the **Objective Function** tab has the following options:

File Icons

- The **[Load from DB]** icon reloads all the observation groups from the database
- The **[Save to DB]** icon saves any changes to the observation groups to the database

Measurement Icons



- The **[Heads]** icon lists all the head observation groups
- The **[Concentration]** icon lists all concentration observation groups
- The **[Zone Budget]** icon lists all the zone budget observation groups.

User Group Icons

- The **[Edit Selected User Group]** icon edits a group created by the user. To edit the group, it must be highlighted.
- The **[Create New User Group]** icon allows the user to create a new group.
- The **[Delete Selected User Group(s)]** icon deletes a group created by the user. To delete the group, it must be highlighted.

Group Icons

Visual MODFLOW creates three different groups of observations:

- **Well Groups** containing observation points from each well
- **Layer Groups** containing observations for each model layer
- **User Groups** containing user-defined observation groups

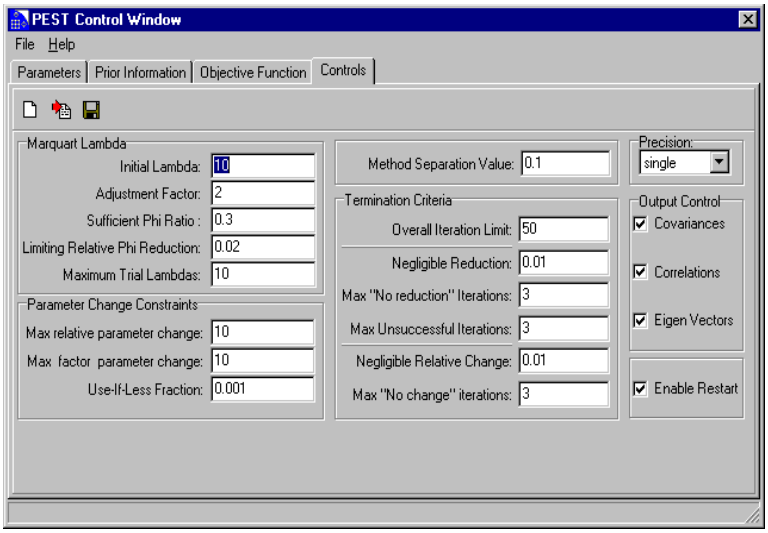
The Group icons control which observation groups are included in the Groups list. By default, all Observation groups are listed.

When a group is selected (indicated by a ✓in its respective checkbox), any group intersecting with that group are checked and then greyed out because PEST does not allow an observation to belong to more than one group.

4.5.4 Setting PEST Control Parameters

The PEST **Controls** tab is used to modify any of the default values for the PEST controls. These variables are described in detail in Chapter 4 of the WinPEST User's Manual.

Once all of the PEST Control information has been defined, select **File** and then **Save & Exit** from the top pull-down menu to save this information and return to the **Run** section of Visual MODFLOW.



4.6 Running the Model

One of the benefits of Visual MODFLOW is the seamless integration with all of the numeric engines including:

- MODFLOW 96 and MODFLOW 2000
- MODPATH
- Zone Budget
- MT3Dv.1.5, MT3DMS, MT3D96, MT3D99 and RT3D
- PEST

The seamless integration with each of these is accomplished through a program called VM Engine, containing 32-bit, native Windows versions of each numeric engine. The VM Engine program is started by Visual MODFLOW but it is run as a separate program outside of the Visual MODFLOW environment.

To run a simulation with any or all of the above numeric engines, select **Run** from the top menu bar of the **Run** section and the **Engines to Run** dialog will appear as shown in the following figure.

The **Engine** column lists the available numeric engines, and the **Run** column indicates which numeric engines will be run during the simulation. Any or all of the available numeric engines can be run for the simulation provided the required data files are present in the model project folder.

The **MODFLOW** engine can be run by itself without any requirements from any of the other engines.

The **MODPATH** engine requires a valid .BGT file to be present in the project folder. This file will be automatically created if MODFLOW and MODPATH are mutually selected.

The **Zone Budget** engine requires a valid .BGT file to be present in the project folder. This file will be automatically created if MODFLOW and MODPATH are mutually selected.

The **MT3D** engine requires a valid .FLO file to be present in the project folder. This file will be automatically created if MODFLOW and MT3D are mutually selected.

The **PEST** engine must be run with **MODFLOW** and can optionally be run with **MT3D**.

The **[Translate & Run]** button will translate the model input data from Visual MODFLOW file formats to the data files required for the selected numeric engines (see Appendix A) and then start the VM Engine program to run the simulations.

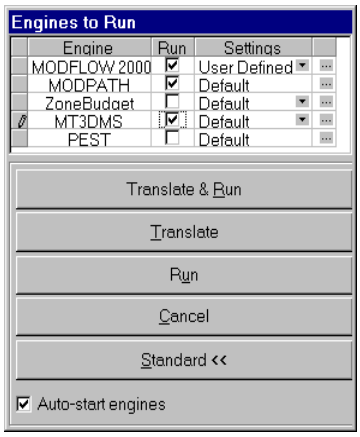
The **[Translate]** button will translate the model input data from Visual MODFLOW file formats to the data files required for the selected numeric engines (see Appendix A).

The **[Run]** button will start the VM Engine program and run the selected numeric engines using the required data files already present in the project folder. If the required files are not present in the project folder, the numeric engines will not run. A warning message will appear indicating that the Visual MODFLOW files will not be translated prior to running the model. Press the **[OK]** button to start the simulation.

The **[Cancel]** button will close the **Engines to Run** dialog without translating or running any model files.

The **[Advanced]** button will expand the **Engines to Run** dialog to include a **Settings** column indicating either **Default** or **User Defined** setting as shown in the following figure. This setting is primarily used to control the **Translate** and **Run** options for the individual data sets associated with the **MODFLOW**, **Zone Budget** and **MT3D** engines.

The **Auto-Start Engines** option indicates whether the selected numeric engines will automatically start running the simulation when the **[Translate & Run]** button is selected or when the **[Run]** button is selected. If this option is selected, then VM Engines will automatically start running the simulation when it opens. If this option is not selected, VM Engines will open with the current simulation loaded, but it will not automatically start the simulation. This option is usually disabled in order to prepare a batch.



Advanced MODFLOW Run Settings

MODFLOW was originally developed in a modular format to make it easy to incorporate different model elements such as Rivers, Streams, Recharge and Evapotranspiration. The code for each of these elements was developed as add-on “packages” for the MODFLOW program, and the data for each of these packages are stored in separate files.

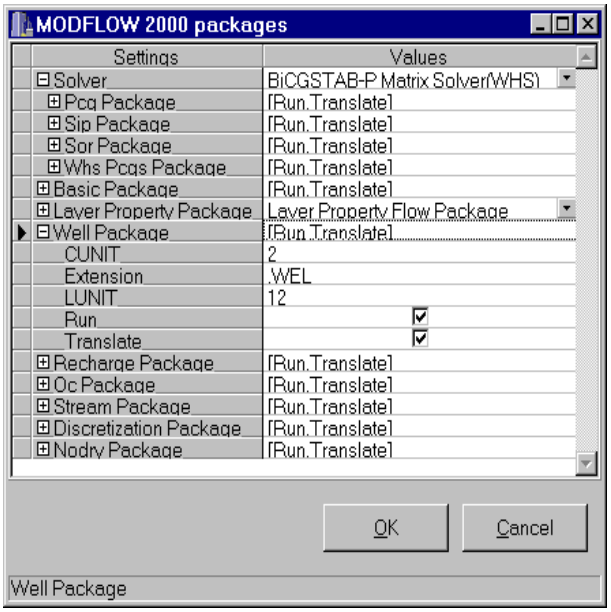
The **Default** setting will translate and run ALL of the relevant Visual MODFLOW data required to create ALL of the input data sets required by the select numeric engines.

The **User Defined** run setting for MODFLOW can be used to disable selected MODFLOW packages so they will not run during the current simulation, or these settings can be used to prevent Visual MODFLOW from creating input files for selected packages.

This option is useful in situation where Visual MODFLOW does not provide the options required to produce the type of input configuration desired for one of the packages. If the MODFLOW input file is created outside of the Visual MODFLOW environment, then Visual MODFLOW needs to be instructed to run this file but NOT to create (translate) this file during the translation process.

Click the **[...]** button in the **MODFLOW Setting** column to load the **MODFLOW Packages** dialog as shown in the following figure.

Each of the available MODFLOW packages for the current model is listed.



Click the **[+]** button to view the parameter settings for each pack**age. The CUNIT, Extension and LUNIT** values are read-only, while the **Run** and **Translate** checkboxes can be modified to activate/disable selected MODFLOW packages.

The minimum set of packages required by MODFLOW is the Basic Package (.BAS), the Block Centered Flow Package (.BCF), the Output Control Package (.OC) and one of the Solver Packages (PCG, .SIP or .SOR). These packages must always be run for each MODFLOW simulation, but they do not necessarily need to be translated (created) by Visual MODFLOW.

Running Input Files From Unsupported Packages

When the **MODFLOW packages** window is opened, Visual MODFLOW checks the project directory for model input data files from MODFLOW packages not currently support by the Visual MODFLOW graphical interface. These files include:

- *projectname*.ETS (Evapotranspiration with a segmented function)
- *projectname*.DRT (Drains with a return flow)
- *projectname*.LAK (Lakes)
- *projectname*.FHB (Flux and Head)
- *projectname*.RES (Reservoir)

If one of these MODFLOW input files are detected in the Visual MODFLOW project directory, it will be listed in the **MODFLOW packages** window and the default **Setting** for the package(s) will be to **Run** this input file with the model simulation.

Substituting Input Files

In some circumstances Visual MODFLOW may not have all of the appropriate graphical or data manipulation tools required to produce the desired distribution of data. In these circumstances it may be necessary to write a FORTRAN or Visual Basic program to manipulate or create the required MODFLOW input files. Visual MODFLOW can still run these input files but the **Translate** option needs to be disabled for the selected MODFLOW Package input files being generated outside of Visual MODFLOW. This will prevent Visual MODFLOW from creating this input file, but if

the Run option is still selected, the model will use the externally generated input file as long as it is located in the same directory as the Visual MODFLOW model.

Advanced Zone Budget Run Settings

The ZoneBudget program reads the MODFLOW output and calculates a water budget between user-defined zones and other zones automatically identified by Visual MODFLOW.

Typically, water budget zones are defined in order to aid in the calibration of the model (e.g. determine how much water is exiting the model through a constant head boundary). Visual MODFLOW automatically assigns a zone number to the various conductivity zones and boundary conditions.

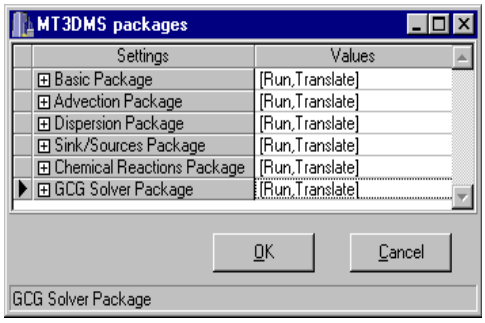
Advanced MT3D Run Settings

Similar to MODFLOW, MT3D was also developed in a modular format to incorporate different model elements including source terms and reactions. The code for these elements was developed as add-on “packages” for the MT3D program, and the data for each of these packages are stored in separate files.

The **User Defined** run setting for MT3D can be used to disable selected MT3D packages so they will not run during the current simulation, or these settings can be used to prevent Visual MODFLOW from creating input files for the selected packages.

This option is useful in situation where Visual MODFLOW does not provide the options required to produce the type of input configuration desired for one of the packages. If the MT3D input file is created outside of the Visual MODFLOW environment, then Visual MODFLOW needs to be instructed to run this file but NOT to create (translate) this file during the translation process.

Click the browse **[...]** button in the **MT3D Setting** column to load the **MT3D Packages** dialog as shown in the following figure.



Each of the available MT3D packages for the current model is listed.

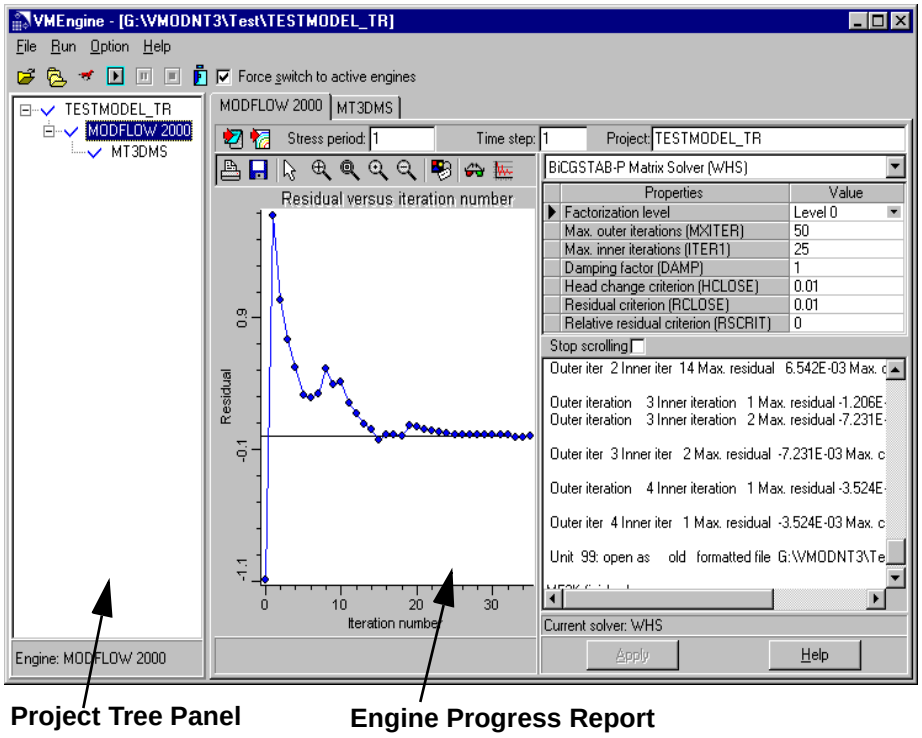
Click the **[+]** button to view the parameter settings for each pack**age. The CUNIT, Extension and** LUNIT values are read-only, while the **Run** and **Translate** checkboxes can be modified to activate/ disable selected MODFLOW packages.

The minimum set of packages required by MT3D is the Basic Transport Package (.BT3) and the Advection Package (.AD3), the Output Control Package (.OC) and one of the Solver Packages (PCG, .SIP or .SOR). These packages must always be run for

each MT3D simulation, but they do not necessarily need to be translated (created) by Visual MODFLOW.

4.6.1 VM Engines

VM Engines provides the numeric 'horsepower' for Visual MODFLOW. It contains all of the numeric engines support by Visual MODFLOW (MODFLOW, MODPATH, Zone Budget, and MT3D) compiled and optimized to run as 32-bit native Windows applications. Although VM Engines is run in a separate window outside of the Visual MODFLOW environment, it is seamlessly integrated with Visual MODFLOW through the **Run** section. The VM Engines program can only be started from the **Engines to Run** dialog by selecting the **[Translate & Run]** button or the **[Run]** button as discussed in the previous section. The **VM Engines** window is shown in the following figure.



The **Project Tree** lists the model(s) currently loaded in VM Engines and the numeric engines associated with each model.

The **Engine Progress Report** displays a real-time graphical progress report for the numeric engine that is currently running. A separate tab will be created for each numeric engine associated with each project.

If the **Force switch to active engine** option is selected, the Engine Progress Report tab will automatically switch to display the report for the engine that is currently running. However, if VM Engines is being used as a batch processor to sequentially run multiple projects, the constant switching makes it difficult to analyze the report from a particular run and may become annoying. To stop the constant switching to each active engine simply disable this option.

Opening New Projects

To load a new project model into VM Engines, select **File/New Project** from the top menu bar and then select the new project model (.VMF). This project will replace the current project(s) in VM Engines.

Adding Projects

To open an additional project models into VM Engines, select **File/Add Project** from the top menu bar of the VM Engines window and then select the new project model (.VMF). This project will be appended to the list of projects in the **Project Tree**.

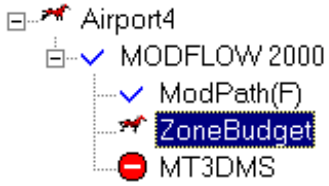
Deleting Project and Engines

To delete a project or individual numeric engines from the **Project Tree**, right-click on the item to delete and select the **Delete** option.

Running the Model(s)

If the **Auto-Start Engines** option is selected in the **Engines to Run** dialog, the current project model will automatically open in VM Engines and start running the selected numeric engine(s).

A red horse symbol beside the project name indicates the model simulation is currently running,



- A blue checkmark beside the project name indicates the model simulation is complete.
- A red horse symbol beside the numeric engine indicates which engine is currently running,
- A blue checkmark beside the engine indicates it is completed
- A red circle beside the engine indicates it is waiting for the preceding engines to complete before it starts running,
- A red X indicates the model has stopped and was not able to run to completion.

Run Selected Project

If the **Auto-Start Engine** option is not active, the simulation runs for a selected project can be started by selecting **Run/Run *projectname*** from the top menu bar of the **VM Engines** window, or by clicking the **Run project** icon above the **Project Tree**.

Run All Projects

If more than one project is loaded in VM Engines, all of the projects can be run in succession by selecting **Run/Run All Projects** from the top menu bar of the **VM Engines** window, or by clicking the **Run All Projects** icon above the **Project Tree**.

Pausing the Running Engine

The numeric engine currently running in VM Engines can be paused by selecting **Run/Pause** from the top menu bar of the **VM Engines** window, or by clicking the **Pause** icons above the **Project Tree**. To restart the simulation, press the **Resume** project icon.

Stopping the Project Run

The current simulation can be terminated by selecting **Run/Terminate** from the top menu bar of the **VM Engines** window, or by clicking the **Stop** icon above the **Project Tree Panel**.

Batch Run Simulations

Multiple modeling projects can be loaded into VM Engines for the purpose of starting a batch run of simulations. To add a project to VM Engines select **File/Add Project** from the top menu bar of the VM Engines window and then select the project model file (*projectname*.VMF). This project will be appended to the list of projects in the **Project Tree**.

> **Note:** The Visual MODFLOW project files selected must be created by the most recent version of Visual MODFLOW before they can be added to the **Project Tree**.

MODFLOW Display Options

The Engine Progress Panel for MODFLOW provides the following functionality:

- display the current stress period and time step for the simulation
- display a graphical progress report of the solution convergence data (maximum residual head vs. number of iterations)
- display the current solver being used and the associated parameters
- display a text-based report of the solution progress for each solver iteration
- on-the-fly modification of the solver and solver parameters
- display a preview of contour maps and color maps of the head and drawdown distributions

The appearance of the graphical display of the residuals graph can be modified using the toolbar above the graph. The display options and properties of this graph are described in Chapter 7.

Modifying Solver Parameters

The selected solver and associated convergence criteria are displayed on the right hand side of the MODFLOW **Engine Progress Panel**. These settings were defined in the Run section of Visual MODFLOW prior to running the simulation. However, if the solution is encountering some difficulties in converging (as is often the case with complex multi-layered models) it may be necessary to adjust the convergence criteria during certain times of the simulation, or perhaps to even switch solvers.

Any changes to the solver parameters will take effect once the **[Apply]** button is pressed. Some of the parameters can be updated after each iteration and will take effect immediately, while other parameters require the simulation to restart from the beginning. The following parameter changes will cause MODFLOW to restart:

PCG2

- Changing to a different solver
- Maximum number of outer iterations
- Maximum number of inner iterations
- Preconditioning method

SIP

- Changing to a different solver
- Maximum number of iterations
- Preconditioning method

SOR

- Changing to a different solver
- Maximum number of iterations

WHS Solver

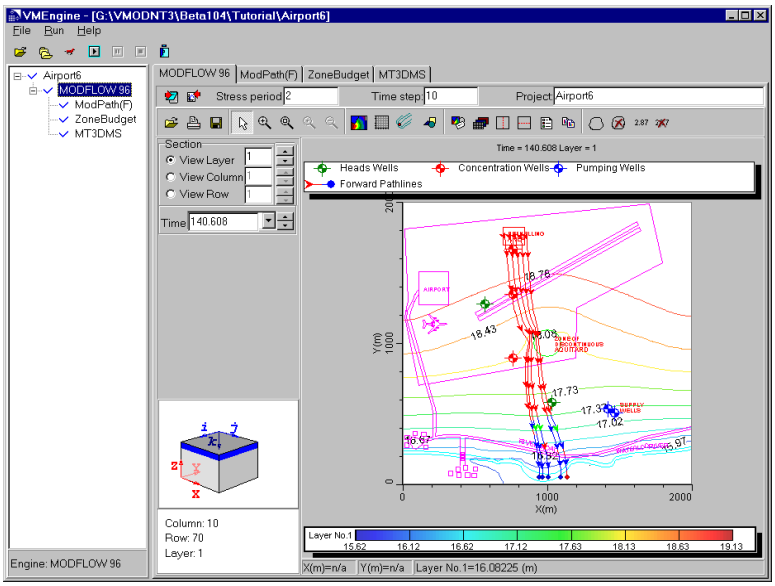
- Changing to a different solver
- Maximum number of outer iterations
- Maximum number of inner iterations
- Factorization level

If MODFLOW must restart a warning message will appear, "**Changing this solver parameter will result in restart of MODFLOW. Proceed?**". Select the **[Yes]** button to restart the MODFLOW simulation.

MODFLOW Output Preview

Once the MODFLOW simulation has run to completion, the **Show Output** icon at the top of the **MODFLOW Progress Report** will become active. Click this icon to switch

from the **MODFLOW Progress Report** to the **Output Preview** as shown in the following figure.

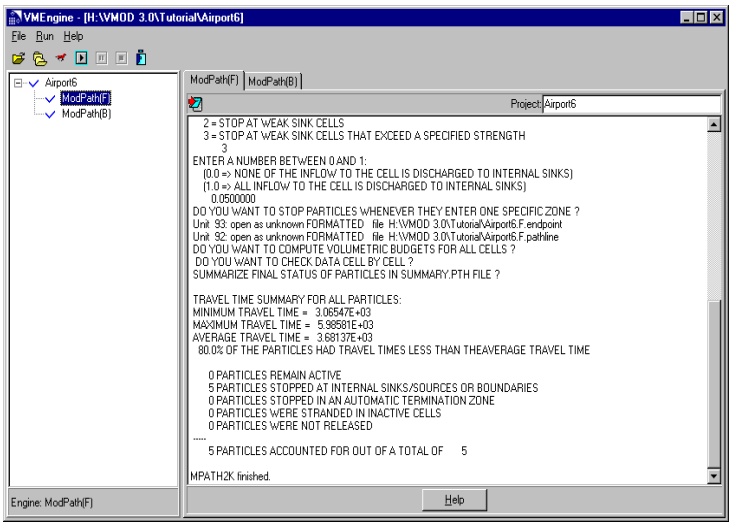


The **Output Preview** displays a contour map of the model heads together with a site map (and pathlines if applicable). The appearance properties of this map view are described in Chapter 7.

Click the **Progress Report** icon to return to the **MODFLOW Progress Report**.

MODPATH Display Options

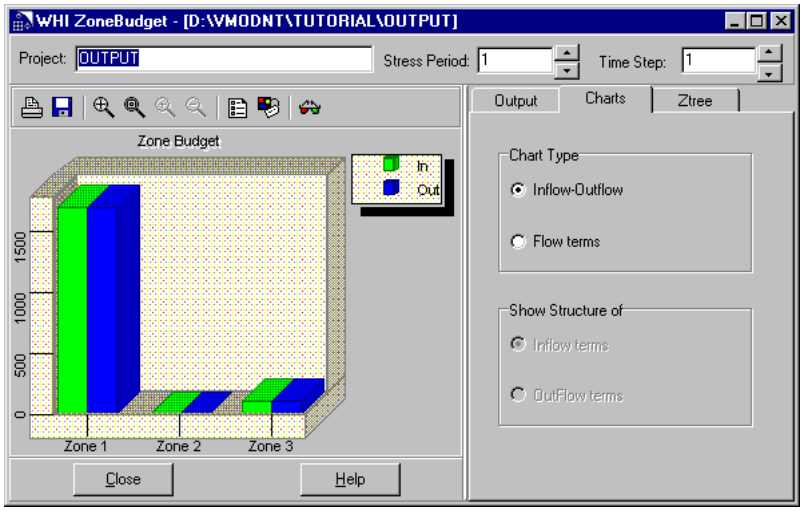
The **MODPATH Progress Report** displays information similar to the following figure.


VMEngine - [H:\VMOD 3.0\Tutorial\Airport6]
File Run Help
Airport6
ModPath(F)
ModPath(B)
ModPath(F) ModPath(B)
Project: Airport6
2 = STOP AT WEAK SINK CELLS
3 = STOP AT WEAK SINK CELLS THAT EXCEED A SPECIFIED STRENGTH
3
ENTER A NUMBER BETWEEN 0 AND 1:
(0.0 => NONE OF THE INFLOW TO THE CELL IS DISCHARGED TO INTERNAL SINKS)
(1.0 => ALL INFLOW TO THE CELL IS DISCHARGED TO INTERNAL SINKS)
0.0500000
DO YOU WANT TO STOP PARTICLES WHENEVER THEY ENTER ONE SPECIFIC ZONE ?
Unit 93: open as unknown FORMATTED file H:\VMOD 3.0\Tutorial\Airport6.F.endpoint
Unit 92: open as unknown FORMATTED file H:\VMOD 3.0\Tutorial\Airport6.F.pathline
DO YOU WANT TO COMPUTE VOLUMETRIC BUDGETS FOR ALL CELLS ?
DO YOU WANT TO CHECK DATA CELL BY CELL ?
SUMMARIZE FINAL STATUS OF PARTICLES IN SUMMARY.PTH FILE ?
TRAVEL TIME SUMMARY FOR ALL PARTICLES:
MINIMUM TRAVEL TIME = 3.06547E+03
MAXIMUM TRAVEL TIME = 5.98581E+03
AVERAGE TRAVEL TIME = 3.68137E+03
80.0% OF THE PARTICLES HAD TRAVEL TIMES LESS THAN THEAVERAGE TRAVEL TIME
0 PARTICLES REMAIN ACTIVE
5 PARTICLES STOPPED AT INTERNAL SINKS/SOURCES OR BOUNDARIES
0 PARTICLES STOPPED IN AN AUTOMATIC TERMINATION ZONE
0 PARTICLES WERE STRANDED IN INACTIVE CELLS
0 PARTICLES WERE NOT RELEASED
5 PARTICLES ACCOUNTED FOR OUT OF A TOTAL OF 5
MPATH2K finished.
Engine: ModPath(F)
Help

This window displays the results and progress of the MODPATH calculations. It also provides a travel time summary for all particles and an explanation of where each particle became inactive or stopped in the simulation.

Zone Budget Options

The **Zone Budget Progress Report** provides a real-time graphical display of the Zone Budget results as they are calculated.



At the top of the screen is the project name of the model and the current stress period and time step being displayed on the chart. The chart may display either accumulative

flows into or out of the aquifer or it may display individual flow rates (constant heads, rivers, etc.). The appearance settings for the graph are described in Chapter 7.

On the right side of the screen are three tabs:

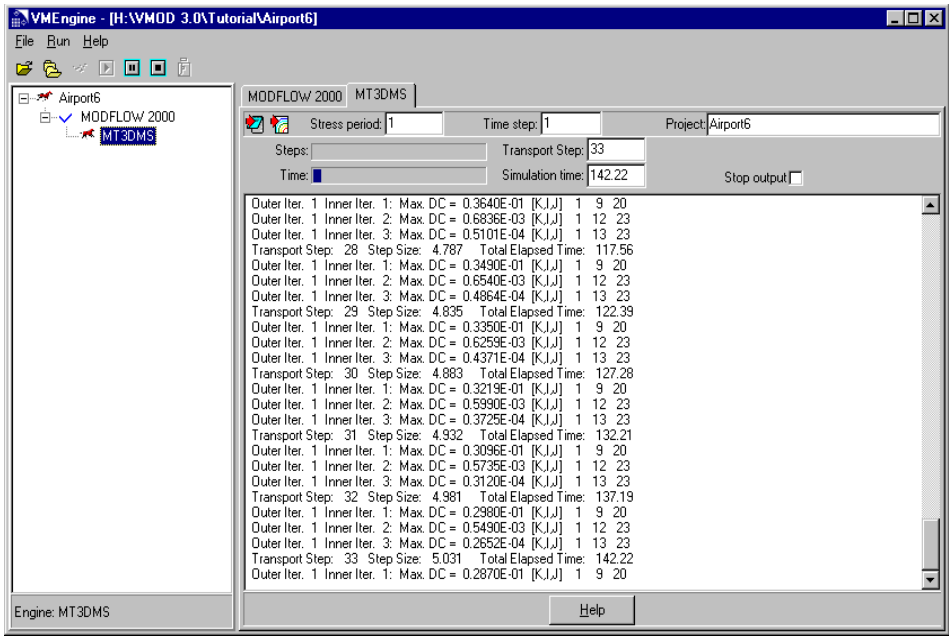
Output Displays a summary of events during the Zone Budget calculations including input and output files

Charts Select the type of data to display in the graph. The **Inflow-Outflow** option will display the Total Inflow value and Total Outflow value for the entire model at each output time step, while the **Flow Terms** option will display either the Inflow values or the Outflow values for each active boundary condition type and Storage terms as they apply to each user-defined zone.

Ztree Select the stress period, time steps, zones and corresponding zone flow rates that are viewed on the chart. The **Ztree** is a directory tree with stress periods as the main branches. Each stress period can be expanded to show corresponding time steps, zones, and flow rates, in that order.

MT3D Display Options

The information reported in the MT3D/RT3D window will appear differently depending on the Advection method selected and whether or not the GCG solver has been selected. However, the **MT3D Progress Report** should appear similar to the following figure.


VMEngine - [H:\VMOD 3.0\Tutorial\Airport6]
File Run Help
Airport6
MODFLOW 2000
MT3DMS
MODFLOW 2000 MT3DMS
Stress period: 1
Time step: 1
Project: Airport6
Steps:
Transport Step: 33
Time:
Simulation time: 142.22
Stop output
Outer Iter. 1 Inner Iter. 1: Max. DC = 0.3640E-01 [K,I,J] 1 9 20
Outer Iter. 1 Inner Iter. 2: Max. DC = 0.6836E-03 [K,I,J] 1 12 23
Outer Iter. 1 Inner Iter. 3: Max. DC = 0.5101E-04 [K,I,J] 1 13 23
Transport Step: 28 Step Size: 4.787 Total Elapsed Time: 117.56
Outer Iter. 1 Inner Iter. 1: Max. DC = 0.3490E-01 [K,I,J] 1 9 20
Outer Iter. 1 Inner Iter. 2: Max. DC = 0.6540E-03 [K,I,J] 1 12 23
Outer Iter. 1 Inner Iter. 3: Max. DC = 0.4864E-04 [K,I,J] 1 13 23
Transport Step: 29 Step Size: 4.835 Total Elapsed Time: 122.39
Outer Iter. 1 Inner Iter. 1: Max. DC = 0.3350E-01 [K,I,J] 1 9 20
Outer Iter. 1 Inner Iter. 2: Max. DC = 0.6259E-03 [K,I,J] 1 12 23
Outer Iter. 1 Inner Iter. 3: Max. DC = 0.4371E-04 [K,I,J] 1 13 23
Transport Step: 30 Step Size: 4.883 Total Elapsed Time: 127.28
Outer Iter. 1 Inner Iter. 1: Max. DC = 0.3219E-01 [K,I,J] 1 9 20
Outer Iter. 1 Inner Iter. 2: Max. DC = 0.5990E-03 [K,I,J] 1 12 23
Outer Iter. 1 Inner Iter. 3: Max. DC = 0.3725E-04 [K,I,J] 1 13 23
Transport Step: 31 Step Size: 4.932 Total Elapsed Time: 132.21
Outer Iter. 1 Inner Iter. 1: Max. DC = 0.3096E-01 [K,I,J] 1 9 20
Outer Iter. 1 Inner Iter. 2: Max. DC = 0.5735E-03 [K,I,J] 1 12 23
Outer Iter. 1 Inner Iter. 3: Max. DC = 0.3120E-04 [K,I,J] 1 13 23
Transport Step: 32 Step Size: 4.981 Total Elapsed Time: 137.19
Outer Iter. 1 Inner Iter. 1: Max. DC = 0.2980E-01 [K,I,J] 1 9 20
Outer Iter. 1 Inner Iter. 2: Max. DC = 0.5490E-03 [K,I,J] 1 12 23
Outer Iter. 1 Inner Iter. 3: Max. DC = 0.2652E-04 [K,I,J] 1 13 23
Transport Step: 33 Step Size: 5.031 Total Elapsed Time: 142.22
Outer Iter. 1 Inner Iter. 1: Max. DC = 0.2870E-01 [K,I,J] 1 9 20
Engine: MT3DMS
Help

As the MT3D run progresses, the **Stress period**, **Time step**, **Elapsed time** and **Simulation time** are displayed. The **Steps** progress bar displays the percentage of transport steps, out of the maximum allowable number of transport steps, used so far. The **Time** progress bar indicates how much of the total simulation time has been simulated.

MT3D Output Preview

In many cases the computation time required for a single contaminant transport simulation can take hours or even days to run to completion. This is a long time to wait just to discover something was obviously wrong with the simulation, particularly when this could have been detected during one of the early output times. This is why VM Engines provides the ability to preview the MT3D simulation results after each output time.

Once the first output time has been calculated, click the **[Show Output]** button in the **MT3D Progress Report Panel** to switch to the **MT3D Output Preview Panel** shown below.

The **MT3D Output Preview Panel** displays a concentration contour map for the first species listed in the model. If the simulation contains multiple species, right-click on the graph to choose which species to display. The appearance properties of this map view are described in Chapter 7.

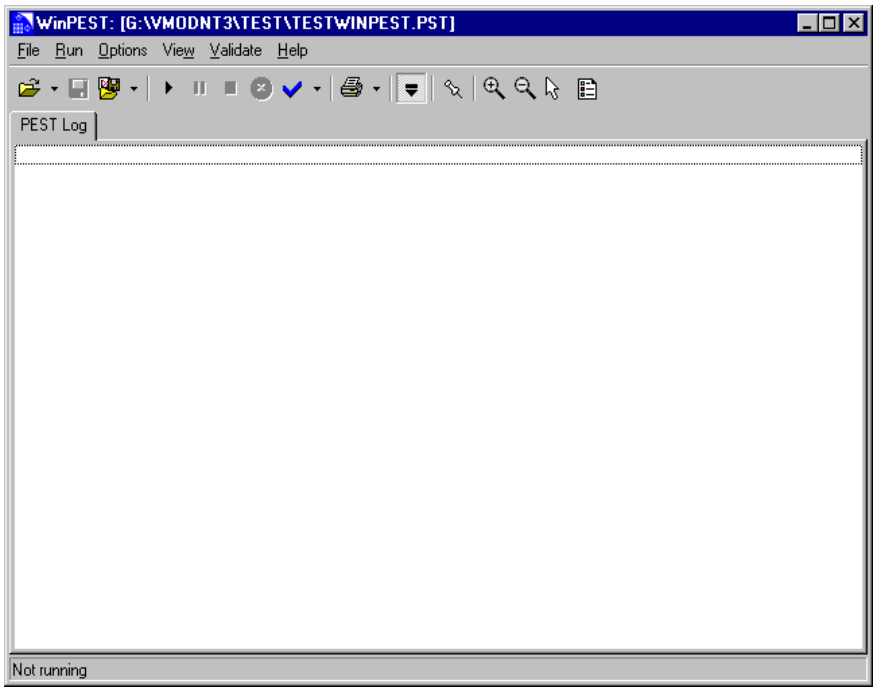
Click the **Progress Report** icon to return to the **MT3D Progress Report Panel**.

4.7 Running Parameter Estimation using WinPEST

Parameter estimation can be run directly from Visual MODFLOW using WinPEST (this requires the WinPEST add-on for Visual MODFLOW). The setup of the parameter estimation input is described in section PEST Run Settings on page 202.

To run the parameter estimation simulations using WinPEST, the **PEST** engine must be selected in the **Engines to run** window (see section Running the Model on page 209).

Once the file translations are completed, the WinPEST window will appear as shown in the following figure.



WinPEST is the Windows command centre for the PEST simulation. **WinPEST** is a graphical interface for starting, controlling, displaying and interpreting the PEST simulation processes including:

- Loading PEST input files
- Validating PEST input data
- Starting (or restarting) the PEST simulation
- Interacting with the PEST simulation (hold parameters)
- Displaying and saving graphical reports of the PEST analysis data and results

When the PEST simulation is run directly from Visual MODFLOW, all of the required PEST input files are automatically prepared by Visual MODFLOW and loaded into WinPEST. As a result, the PEST simulation can be started immediately by selecting the

Run/Start/Start new run option from the top menu bar, or by pressing the **[Run project]** icon on the toolbar.

The following sections provide a brief description of the WinPEST interface, features and functionality. A more detailed description of WinPEST is available in the WinPEST User's Manual provided with Visual MODFLOW.

4.7.1 Loading PEST Input Files

As mentioned previously, if PEST is run directly from Visual MODFLOW, all of the PEST input files are automatically prepared and loaded into WinPEST. However, alternative PEST input files may also be loaded and run if they are prepared using the proper formats.

To load a PEST Control file for the current project, select **File/Open/Project** from the top menu bar or click the **Open PEST control file** icon from the toolbar.

To load a completely new project and all associated PEST input files, select **File/Open/File** and open one each of the following PEST input files: Control file (***.**PST), Parameter Hold file (***.**HLD), Template file (***.**TPL), Parameter file (***.**PAR), or Instruction file (***.**INS).

To load the graphs from the results of a previous PEST simulation, select **File/Load graphs** from the top menu bar, and choose either **Current plot** or **All plots**.

4.7.2 Validating PEST Input Files

PEST comes with a built-in set of handy data validation utilities for checking the input files to make sure they have the required format. Although the chance of creating invalid data input files is greatly reduced by using Visual MODFLOW, it is probably a good idea to run the data validation checks prior to running the PEST simulation just to avoid any unnecessary complications.

The Validations can be run by selecting **Validate** from the top menu bar (or by clicking the **Check** icon in the toolbar) and choosing one of the options described below. If any problems are encountered PEST will issue error messages to the PEST log screen.

The **Validate/Check all** option will run a check on all of the PEST input files to ensure they have the proper formats and information.

The **Validate/Instructions** option will run a check on the PEST Instructions file (.INS)

The **Validate/Template** option will run a check on the PEST Template file (.TPL)

4.7.3 Starting the PEST Simulation

Once the PEST input files are all loaded and validated, the PEST simulation can be started by selecting **Run/Start/Start new run** from the top menu bar or by clicking the **Run project** icon in the toolbar.

A command line window will open to indicate PEST is running. Do not close this window. If this command line window is closed, the PEST simulation will be terminated.

4.7.4 Interacting with the PEST Simulation

Once the PEST run has started, there are a number of tools available for interacting with simulations.

The PEST simulation can be paused by selecting **Run/Pause** from the top menu bar or by clicking the **Pause** icon in the toolbar.

The PEST simulation can be stopped by selecting **Run/Stop** from the top menu bar or by clicking the **Stop** icon in the toolbar.

Insensitive parameters may be 'held' (frozen) at the current value by selecting **View/ Hold Parameter(s)** from the top menu bar or by clicking the **Hold parameter(s)** icon in the toolbar. A **Hold Status** window will appear with a graph of the available parameters. Select the parameter(s) to hold from the graph and then make any other necessary changes to these parameter groups or settings.

4.7.5 Displaying Reports and Graphs

When the PEST simulation starts running, the simulation progress can be viewed using a variety of reporting and graphing formats.

The **View** option in the top menu bar of WinPEST may be used to select the desired reports and graphs to display.

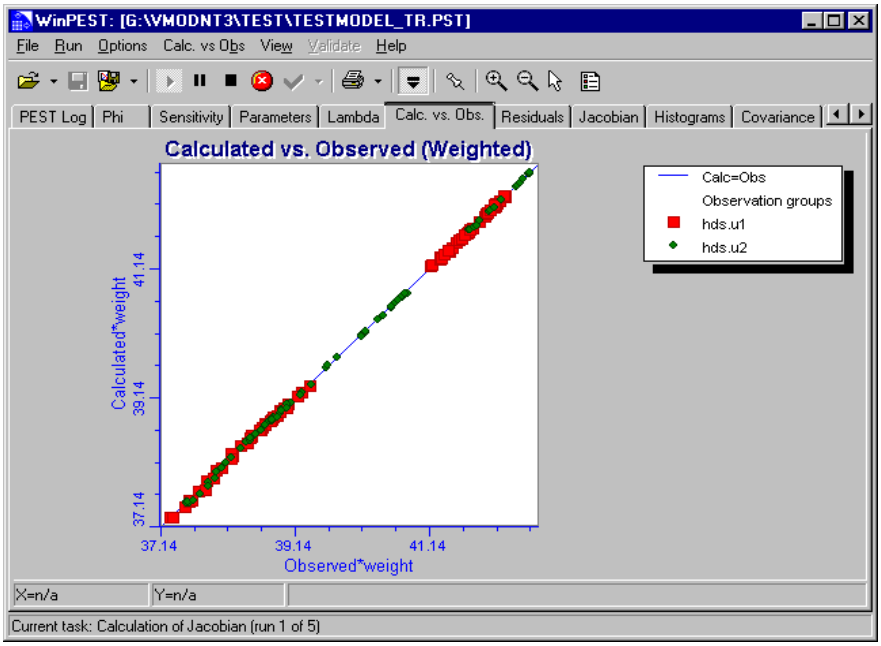
The reports include the PEST Log and the Run Record. The data is written and appended to these reports as the simulation progresses and the reports will automatically scroll down to the bottom to display the most recently added text. The Autoscroll option may be disabled by clicking the **Autoscroll** icon in the toolbar.

A variety of graphs are available for displaying and interpreting the PEST simulation results. These graphs can be selected by choosing the **View/Plots** option in the top menu bar. The available plots to display include:

- **Objective Function**
- **Composite Sensitivity**
- **Parameters History**
- **Marquardt Lambda**
- **Calculated vs. Observed**

- **Jacobian**
- **Correlation**
- **Covariance**
- **Eigenvectors**
- **Eigenvalues**
- **Uncertainties**
- **Residuals**
- **Residual Histogram**
- **Prediction**
- **Regularization Weight Factor**

The displayed graphs will be updated on the fly after each PEST iteration. An example of the Calculated vs. Observed Values graph is shown below.



Once the PEST simulation is completed, the graphs can be saved either as bitmap images to include in a report, or as configuration files to load at a later time. To save the PEST simulation analysis graphs select **File/Save graphs** from the top menu bar and choose either:

- **As picture** to save each plot to a graphics file
- **Current plot** to save only the plot currently being displayed
- **All plots** to save all plots currently being displayed

5

Output Section - Displaying Model Results

The **Output** section of Visual MODFLOW allows the user to visualize, print and export the simulation results. This chapter provides instructions on displaying, interpreting, customizing and printing the groundwater flow, pathline and contaminant transport modeling results using a variety of mapping and graphing presentation formats including:

Map type	**Data type**
Contours	Head, Drawdown and Concentration, Water Table Elevation, Water Table Depth, Head Difference, Flux Between Layers, and Net Recharge
Pathlines	
Velocities	
Zone Budget	
Calibration Residuals	Head and Concentration

Graph Type	**Data type**
Calibration	Head and Concentration
Time Series	Head, Drawdown and Concentration
Mass Balance	Flow and Transport
Zone Budget	Flow and Transport

The Output section of Visual MODFLOW is opened by selecting **Output** from the top menu bar of the **Main Menu**. Upon entering the Output section, Visual MODFLOW will automatically load the available Output files for Head (.HDS), Drawdown (.DDN) and Concentration (.UCN) for all output times. Once these data files are loaded, the Output screen will appear with the following items in the top menu bar.

File	**Save** the settings, **Export** to a graphics file, **Print** the display screen, and return to the **Main Menu**.
Maps	Select a map type to display the modeling results in plan view or cross-sectional view (see list above).
Graphs	Select a graph type to display and interpret the modeling results.
Tools	Open the **Cell Inspector** to view cell-by-cell values, or open the **Annotate** screen to add text, lines, shapes and arrows to the model display area.
Help	Access general information about Visual MODFLOW.

The first time the **Output** section is opened, Visual MODFLOW will display the site map and the head contours for the current layer, row or column. When the **Output** display settings are modified, Visual MODFLOW will always display the most recent Output display settings.

5.1 File Options

The **File** menu options are described as follows:

Save	Save the **Output** settings.
Export	Export the model display area to a graphics file (AutoCAD .DXF or Enhanced Windows Metafile .EMF format), or export the data for the active overlay to an XYZ ASCII .TXT file (in world or model co-ordinates).
Print	Print the screen and select the printer. For more details, please refer to the section Printing Options, found in Chapter 2.
Main Menu	Close the **Output** section and return to the **Main Menu**.

5.2 Maps

Visual MODFLOW displays five different types of maps:

- **Contour** maps
- **Pathlines** maps
- **Velocity Vector** maps
- **Zone Budget** maps
- **Calibration Residual** maps

Each of these map types and the associated display options are presented in the following sections.

5.2.1 Contour Maps

Visual MODFLOW provides a comprehensive selection of contour maps to display contour lines and color maps of selected model parameters including:

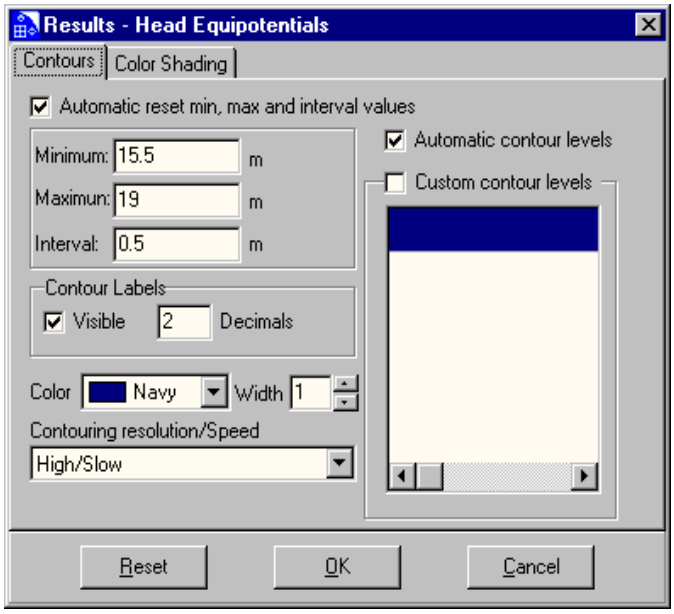
Head	Calculated head values.
Drawdown	Differences between initial head and calculated head.
Concentration	Concentration values for selected chemical species.
Water Table Elevation	Elevation where the calculated head value is equal to the elevation (pressure head equals zero).
Water Table Depth	Depth from the top of layer 1 to the calculated water table elevation.
Head Difference	Differences in calculated head values between layers.
Head Flux	Calculated flux of water between adjacent layers.
Net Recharge	Specified recharge values minus calculated evapotranspiration.

The left-hand toolbar contains several buttons that are present for most of the contour map screens.

[Options]	Customize the contour map and color map appearance settings (see section Contour Map Display Options on page 230).
[Time]	Select the desired output time to display the results.
[Previous]	Display the selected contours for the previous time increment.
[Next]	Display the selected contours for the next time increment.
[Select]	Select observation wells to use for calibration purposes (currently available only for Head, Drawdown and Concentration contour maps).
[Export Layer]	Export the contour data values for the current layer.

Contour Map Display Options

The contour map appearance may be customized by selecting the **[Options]** button from the left-hand toolbar. Depending on the contour map being displayed, a contour options window will appear similar to the following figure with options described below.



- **Automatic reset minimum, maximum and interval values** calculates the default values for the minimum and maximum contour values and the contour interval each time the view is changed (new layer/row/column or output time).
- **Minimum** sets the minimum contour value below which no contour lines will be plotted. This setting is ignored if the **Automatic contour levels** option is not selected.
- **Maximum** sets the maximum contour value above which no contour lines will be plotted. This setting is ignored if the **Automatic contour levels** option is not selected.
- **Interval** sets the contour increment value, starting from the **Minimum** value. This setting is ignored if the **Automatic contour levels** option is not selected.
- **Automatic contour levels** shows/hides the contour line values generated for the **Minimum**, **Maximum** and **Interval** values.
- **Custom contour levels** shows/hides the user-defined contour values indicated in the list
- **Contour Labels** options are used to hide/show the contour labels and to set the number of **Decimals** to plot for each contour line label.
- **Color** sets the color of the contour line

- **Width** sets the width (thickness) of the contour line
- **Contouring resolution/speed** provides a selection of five levels of contour resolution; each level with a corresponding contouring speed (as resolution increases, speed decreases). The **Highest/Slowest** setting uses all grid cells to calculate the contour line location. The **High/Slow** setting takes a representative value from each group of four grid cells. The **Medium/Medium** setting takes a representative value from a group of eight grid cells.

Adding Contour Lines

Contour lines may be added at custom contour levels by selecting the **[Options]** button on the left-hand toolbar and entering the desired **Custom contour levels,** or by right-clicking the mouse pointer on the model domain, choosing the **Add contour(s)** option and then clicking the mouse pointer at the desired location of the contour line(s). A contour line will be plotted at each location corresponding the data value at the selected location(s). These contour lines values will be added to the **Custom contour levels** table in the **Contour** options tab.

Right-click the mouse pointer on the model domain again to stop adding custom contour lines.

Deleting Contour Lines

Custom contour lines can be deleted by selecting the **[Options]** button on the left-hand toolbar and deleting the values from the **Custom contour levels** table, or by right-clicking the mouse pointer on the model domain, choosing the **Delete contour(s)** option and then clicking the mouse pointer on the custom contour lines to delete.

Right-click the mouse pointer on the model domain again to stop deleting custom contour lines.

Alternatively, to delete all custom contour lines, right-click on the model domain and select the **Delete all custom** option.

Adding Contour Labels

Labels can be added to any contour line at any location by right-clicking on the model domain and selecting the **Add Label(s)** option, then click the left mouse button on a contour line where a label should be added. If labels are not being added, make sure the desired contour map is the set as the current overlay.

Deleting Contour Labels

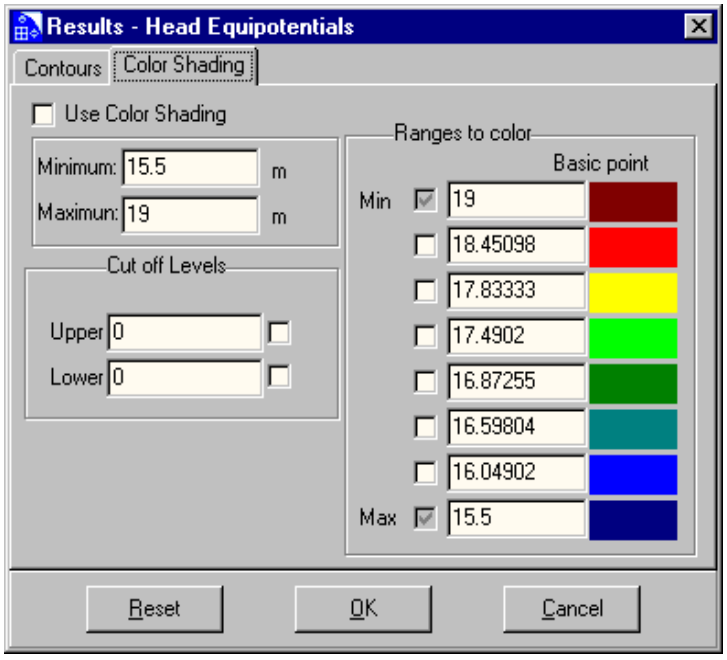
To delete a label, right-click the mouse pointer on the model domain and select the **Delete label(s)** option and click on the label to be deleted.

Moving Labels

Contour line labels can be moved by selecting right-clicking the mouse pointer on the model domain and selecting the **Move Label(s)** option. Then drag-and-drop a selected label to a new location on the same contour line.

Color Map Display Options

The **Color Shading** tab controls the display settings for the color map as shown in the following figure and described below.



- **Use Color Shading** shows/hides the color map
- **Minimum** sets the minimum contour value below which no contour lines will be plotted. This setting is ignored if the **Automatic contour levels** option is not selected.
- **Maximum** sets the maximum contour value above which no contour lines will be plotted. This setting is ignored if the **Automatic contour levels** option is not selected.
- **Ranges to color** indicates the color scale and the data values associated with each color. The **Min.** and **Max.** values are automatically determined by the minimum and maximum data values, respectively, for the selected layer/row/column or output time. The intermediate values are linearly interpolated to each color but may be customized by clicking the checkbox beside the color and entering a new value (the new value must be less than the **Max.** value and

greater than the **Min.** value).

- **Cut off levels** specify the **Upper** and **Lower** limits of the color mapping. Any values above or below the **Upper** and **Lower** limits, respectively, will appear as a solid white color on the model domain. To change these values, click the checkbox beside the field and type the desired value into the corresponding data entry field.

Removing Contour Maps

Once a Contour Map has been selected and displayed in the **Output** section, it can only removed using the **Overlay Control** as described below:

- Press the **[F9 - Overlay]** button in the toolbar along the bottom of the Visual MODLFOW screen to load the **Overlay Control** window.
- Click the **List only the visible overlays** option (this reduces the list of Overlays and makes it easier to locate the Contour Map overlay).
- Locate the Contour Map overlay (looks like "**C(O) - *MapName***") and click the checkbox to remove the checkmark.
- Click the **[OK]** or **[Apply]** button to redraw the model display screen with the new Overlay settings.

Selecting Output Times

Visual MODFLOW runs both steady-state and transient simulations. For steady-state simulations there is only one set of results for each contour map. However, for transient simulations, there may be tens, hundreds or even thousands of output times generated for Head, Drawdown and Concentration results.

To select the output time to display for the current contour map, click the **[Time]** button on the left-hand toolbar and choose the desired output time. Alternatively, the output time displayed may be increased or decreased by pressing the **[Next]** or **[Previous]** button, respectively, located beside the **[Time]** button.

If a Head Contour Map and a Concentration Contour Map are being displayed simultaneously it is important to remember that the Output times for these two data types are not synchronized. As a result, the Output time for the Head Contour Map may be completely different than the Output time for the Concentration Contour Map. Similarly, the Head and Drawdown Output times may also be different.

Selecting Observation Points

During the model calibration process it is often useful to evaluate the model calibration results for selected observation points located in a particular region of interest. The selected Observation Points may then be used to analyze, interpret and plot the model calibration results using a variety of maps, graphs and statistics:

- Calibration Residual Maps (see page 242)
- Calculated vs. Observed Scatter Graphs (see page 244)
- Time-Series Graphs (see page 254)

The **[Select >]** button in the Head and Concentration Contour Map screens is used to graphically select the Head and Concentration Observation Points, respectively.

- **[Select >] All** is used to select all of the Observation Wells in the model.
- **[Select >] None** is used to un-select all of the Observation Wells in the model.
- **[Select >] Single** is used to select in individual Observation Wells by clicking on them.
- **[Select >] Box** is used to select a group of Observation Wells inside the perimeter of a rectangular window. Click the left mouse button at the start corner of the window and then stretch the rectangular window. Click the left mouse button again to close the Window.
- **[Select >] Polygon** is used to select a group of Observation Wells inside the perimeter of a polygon. Click the left mouse button at the start point of the polygon and then click around the perimeter. Click the right mouse button near the start point to close the polygon.
- **[Select >] Group** is used to select all Observation Points belonging to a selected Observation Group.

The green Head Observation Point symbols will be colored blue once they are selected, while the purple Concentration Observation Point symbols will be colored red.

If the model does not contain any Observation Points, then this option can be ignored.

Exporting Contour Data

The modeling results for a selected Output time can be exported to a tab-delimited ASCII data file for viewing or post-processing using a third-party graphics software package.

Exporting Data For Current Layer

The contour data for the current layer may be exported to a text file by selecting the **[Export Layer >]** button from the left-hand toolbar and choosing either:

- **All Cells** to export values for each cell in the current layer (inactive cells and dry cells are assigned head values of 1.0e+30 and 1.0e-30, respectively), or
- **Active Only** to export data only for the active cells in the current layer

The data for the selected layer may be exported to either:

- Tab-separated ASCII text files containing three columns of data {X, Y, Value} where X and Y are the X-coordinate and Y-coordinate for the centre of each grid cell in either a World or Model Co-ordinate system.
- TecPlot data files in either a World or Model Co-ordinate system

If the model is currently being viewed by row or column then the **[Export Layer]** option can not be used.

Exporting Data For All Layers

To export the contour data for the selected Output time to a text file,

- Select **File/Export...** from the top menu bar
- An **Export to file** window will appear
- Select the **XYZ ASCII File type** and enter the **File name**
- Click the **[Save]** button

Contour data such as Head, Concentration, Drawdown, Water Table Elevation, etc. will be exported to an ASCII text file with the following format:

```
X     Y     Z     Value
```

Where;

`X` = X co-ordinate of the centre of the grid cell

`Y` = Y co-ordinate of the centre of the grid cell

`Z` = Z co-ordinate of the centre of the grid cell

`Value` = Contour data value for the grid cell

The grid cells are listed in order starting from the top left-hand corner of the bottom layer of the model and incrementing in the X-direction, then in the Y-direction, and then in the Z-direction.

5.2.2 Pathlines Map

The Pathlines Map can be displayed by selecting **Maps/Pathlines** from the **Output** section. The flow pathlines indicate the flow path and travel time of a groundwater particle due to advective groundwater flow (as calculated by MODPATH).

The Pathlines Map is a little different than the other map types because it does not simply represent a “snap-shot” in time, but rather the pathlines represent a historical travel log of groundwater particles. Forward tracking pathlines are used to predict where groundwater is flowing and how long it will take to reach a given location if it starts from a known location at a known time. Backward tracking pathlines are used to predict where groundwater at a given location and time is coming from and how long it took to get there.

Visual MODFLOW provides a variety of display options for customizing the Pathline map. These options are available from the left-hand toolbar and are described below:

[Options] Modify the travel time, color scheme and time marker settings.

[Projections] Show projections of all pathlines through the model.

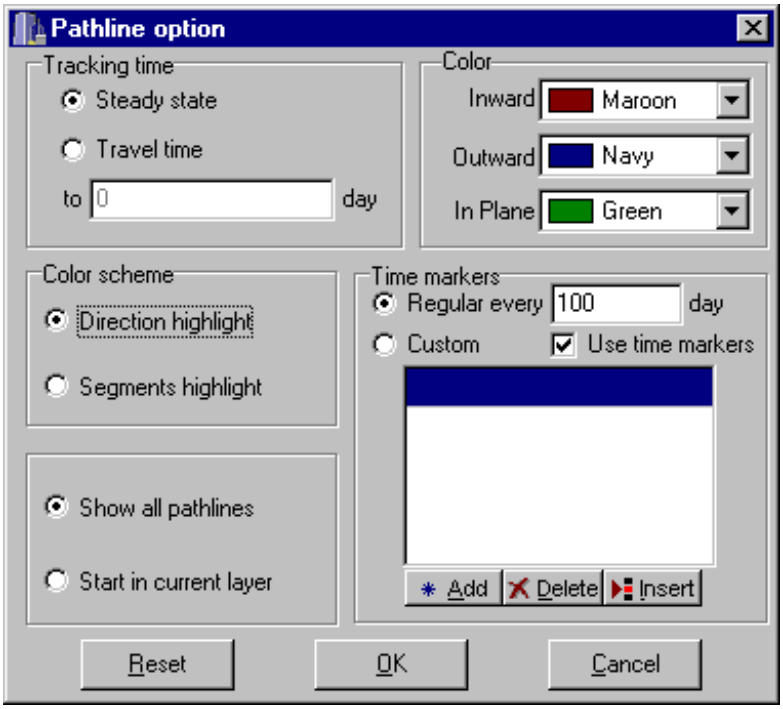
[Segments] Show only those pathlines in the current layer/column/row view.

[Toggle] Toggle pathlines on or off by selecting individual particles or group of particles inside a polygon or box.

By default, when the Pathlines Map is first displayed, all forward and backward pathlines will be displayed in projection view and the entire length of the pathlines will be displayed with time markers and directional color coding.

Pathlines Display Options

Select **[Options]** from the side menu bar and the **Pathline Options** window will appear as shown in the following figure and described below.



- The **Tracking time** option is used to selected either **Steady-state** pathlines for all times, or to specify a maximum **Travel time** for all pathlines.
- The **Color Scheme** option is used to select either **Direction highlight**, where the **Color** of the pathlines are determined by the flow direction relative to the current plane, or **Segments highlight** where the **Color** of the pathlines are determined by their location relative to the current layer.
- **Show all pathlines** displays all the pathlines in all layers/row/columns
- **Start in current layer** displays only pathlines originating in the current layer/ row/column.
- **Colors** defines the colors associated with the selected **Color Scheme**. When

Direction highlight is selected, the **Colors** correspond to pathlines travelling **Inward**, **Outward**, and **In Plane**. When **Segments highlight** is selected the **Colors** correspond to pathlines **Above**, **Below**, and **In Plane**.

- The **Time marker** options are used to hide/show the pathline time markers and to customize the time interval for each time marker. The Time markers can be plotted at **Regular** time intervals or at irregular **Custom i**ntervals.

If forward tracking pathlines do not appear for some particles, check to make sure the particles are not assigned above the water table elevation or in dry cells.

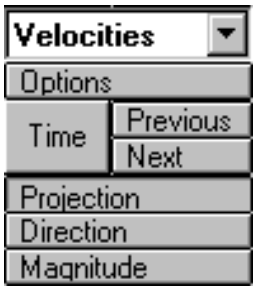
If backward tracking pathlines appear to 'skim' along the surface of the water table instead of exiting through recharge, check the MODPATH **Discharge Options** in the **Run** section to make sure the recharge flux is being assigned to the top face of the all cells instead of being treated as an internal source/sink.

Removing the Pathlines Map

Once the Pathlines Map has been selected and displayed in the **Output** section, it can only removed using the **Overlay Control** as described below:

- Press the **[F9 - Overlay]** button in the toolbar along the bottom of the Visual MODLFOW screen to load the **Overlay Control** window.
- Click the **List only the visible overlays** option (this reduces the list of Overlays and makes it easier to locate the Pathlines Map overlay).
- Locate the **PT - Pathlines** overlay and click the checkbox to remove the checkmark.
- Click the **[OK]** or **[Apply]** button to redraw the model display screen with the new Overlay settings.

5.2.3 Velocity Vector Map



The Velocity Vectors Map can be displayed by selecting **Maps/Velocities** from the **Output** section. The velocity vectors indicate the direction and velocity of groundwater flow throughout the model for a selected output time.

Visual MODFLOW provides a variety of display options on the left-hand toolbar for customizing the Velocity Vector Map.

[Options] Modify the number and scale of Velocity Vectors.

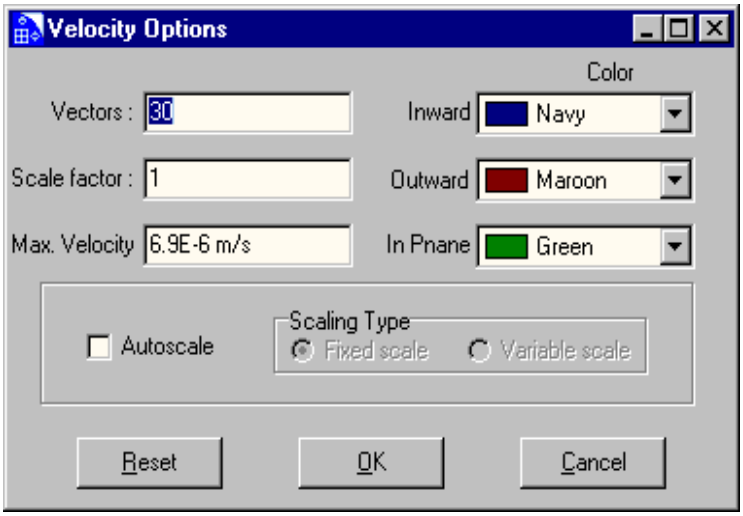
[Projection] View projections of the velocity vectors onto current plane of view.

[Direction] View flow direction vectors (not-to-scale velocity vectors)

[Magnitude] View velocity vectors scaled according to the magnitude of the flow velocity in any direction.

Velocity Vector Display Options

Select **[Options]** from the side menu bar and the **Velocity Options** window appears as shown in the following figure and described below.



This window allows you to select the number of velocity vectors to be displayed and the color of the directional vectors. The following features can be selected:

- **Vectors** is the number of velocity vectors in a row along the longest dimension of the model. The number of velocity vectors along the shorter dimension is calculated to maintain a uniform spacing.
- **Scale factor** is used to set the length of the velocity vector corresponding to the highest flow velocity. This value may need to be increased in order to see the lower range of velocity vectors.
- **Max velocity** indicates the maximum velocity for a vector to be viewed on the model domain.
- **Colors** sets the color codes for the direction of the vectors. The default colors are red for **Outward** vectors, blue for **Inward** vectors, and green for **In plane** vectors.
- **Autoscale** automatically adjusts the size of the velocity vectors depending on the velocities within the current view.
- **Scaling type** provides two auto-scaling options. **Variable scaling** will automatically adjust the velocity vector size such that the vectors do not overlap. **Fixed scaling** does not change the scaling when the number of vectors is changed and some vectors may overlap.

Adding Velocity Vectors

Velocity vectors can be added to the map at selected locations by right-clicking the mouse on the desired location(s). These new velocity vectors can be deleted by pressing the **<Ctrl>** key and right-clicking the mouse on or near the new velocity vector.

Selecting Output Times

Visual MODFLOW runs both steady-state and transient simulations. For steady-state simulations there is only one set of results for each velocity vector map. However, for transient simulations, there may be tens, hundreds or even thousands of output times generated for the flow simulation results.

To select the output time to display for the current velocity vector map, click the **[Time]** button on the left-hand toolbar and choose the desired output time. Alternatively, the output time displayed may be increased or decreased by pressing the **[Next]** or **[Previous]** button, respectively, located beside the **[Time]** button.

If a Head Contour Map and a Velocity Vector Map are being displayed simultaneously the Output times for these two data types will be synchronized because the velocity values are directly dependent on the head values. However, the Velocity Vector Map is not synchronized with the Concentration Contour Maps.

Exporting Flow Velocity Data

The calculated flow velocity for each grid cell in the model at the selected Output time may be exported to an ASCII text file by selecting **File/Export...** from the top menu bar and then choosing the **XYZ ASCII** file format. The velocity data is exported to an ASCII text file with the following format:

X Y Z Vx Vy Vz

Where;

Vx = Velocity in the X-direction (in units of L/T)

Vy = Velocity in the Y-direction (in units of L/T)

Vy = Velocity in the Z-direction (in units of L/T)

Removing the Velocity Vector Map

Once the Velocity Vector Map has been selected and displayed in the **Output** section, it can only removed using the **Overlay Control** as described below:

- Press the **[F9 - Overlay]** button in the toolbar along the bottom of the Visual MODLFOW screen to load the **Overlay Control** window.
- Click the **List only the visible overlays** option (this reduces the list of

Overlays and makes it easier to locate the Velocity Vector Map overlay).

- Locate the **Vel - Vectors** overlay and click the checkbox to remove the checkmark.
- Click the **[OK]** or **[Apply]** button to redraw the model display screen with the new Overlay settings.

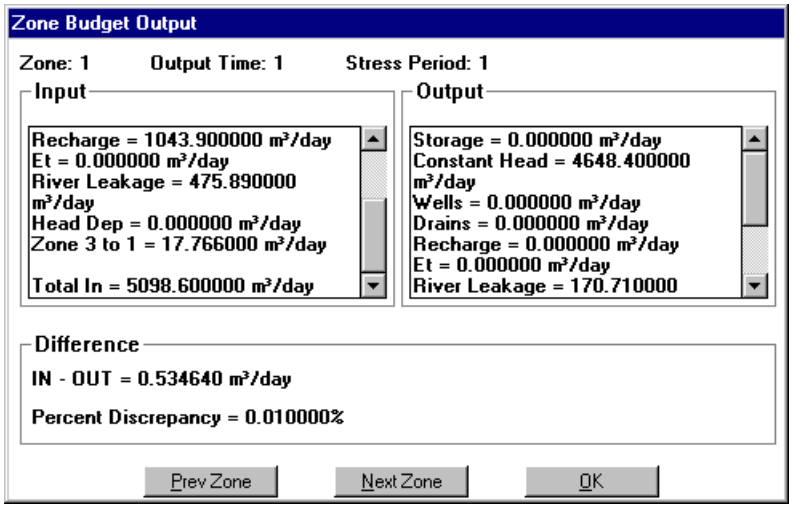
5.2.4 Zone Budget Map

The Zone Budget map displays the various user-defined Zone Budget zones and provides a text-based report of the mass balance results at the end of each stress period, and Zone-to-Zone flow summaries for each Head output time (if Zone Budget was run for the simulation).

The **[Options]** button allows the Zone Budget areas to be shown as **Solid Colors** or as **Outlines**.

Zone Budget Listing

A text-based listing of the Zone Budget results may be presented by pressing the **[Zbud Output]** button on the left-hand toolbar. The following Zone Budget Output window will appear as described below.



The **Zone Budget Output** window details the results of the zone budget calculation for the current time period. By default the output will be for Zone No. 1. Results of any other zones can be displayed by clicking on the **[Prev Zone]** or **[Next Zone]** buttons at the bottom of the window. The output details flow rates (both in and out of the model domain) for each of the following: Constant heads, Drains, Rivers, General Head Boundaries, Recharge, Evapotranspiration, Wells, and Storage.

The **Zone Budget Output** window also indicates accumulative flows into and out of the zone, as well as the percent discrepancy between them.

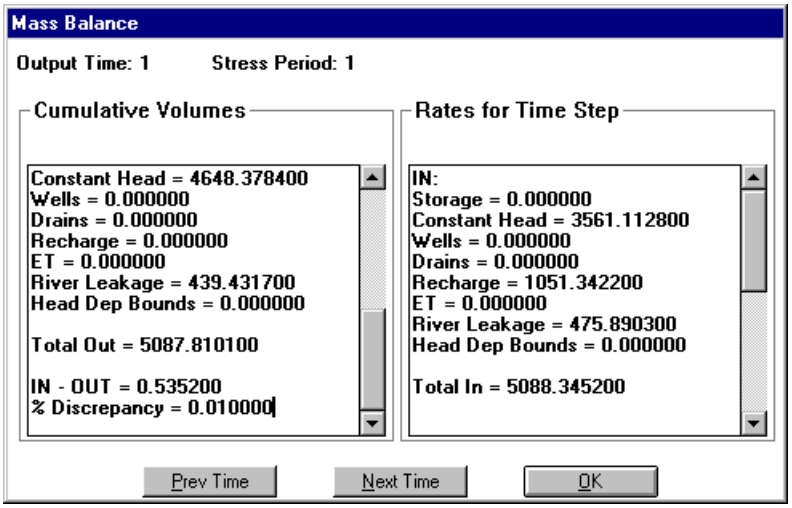
Selecting Output Times

The Zone Budget results for other time periods can be displayed by clicking the **[Time]** button from the left-hand toolbar and selecting the desired Output time, or by pressing the **[Next]** or **[Previous]** buttons to scroll from one output time to the next/previous.

Mass Balance Report

The mass balance is one of the key indicators of a successful simulation. If the mass balance error for a simulation is less than 2% the results of the simulation may be considered to be acceptable provided the model is also calibrated. If the mass balance error is more than 2% then there may be some instabilities in the solution and some inconsistencies in the results.

To see a text-based report of the Mass Balance results, select the **[Mass Balance]** button from the left-hand toolbar and the following **Mass Balance** window will appear as described below.



The **Mass Balance** window details similar information to Zone Budget, except for the entire model domain. Flow rates are given for the same boundaries and properties with accumulative inflows and outflows and a percent discrepancy.

Removing the Zone Budget Maps

Once the Zone Budget Map has been selected and displayed in the **Output** section, it can only removed using the **Overlay Control** as described below:

- Press the **[F9 - Overlay]** button in the toolbar along the bottom of the Visual MODLFOW screen to load the **Overlay Control** window.
- Click the **List only the visible overlays** option (this reduces the list of Overlays and makes it easier to locate the Zone Budget Map overlay).
- Locate the **Gen - Zone Budget** overlay and click the checkbox to remove the checkmark.
- Click the **[OK]** or **[Apply]** button to redraw the model display screen with the new Overlay settings.

5.2.5 Calibration Residual Map

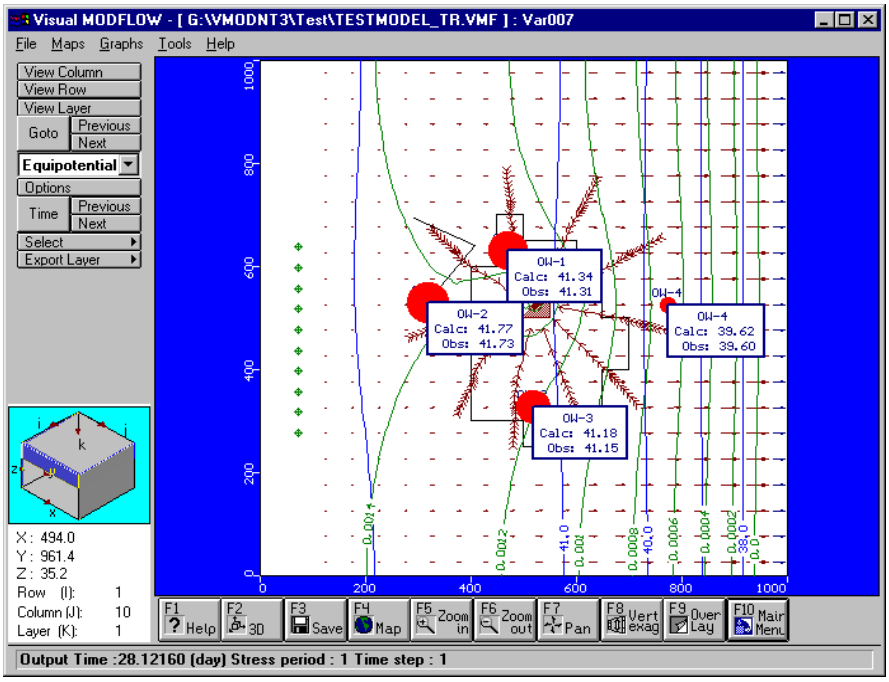
Calibration Residuals are calculated by subtracting the observed values measured at an Observation Point from the Calculated values determined by the model. The value of the Calibration Residual represents a quantitative measure of the 'goodness-of-fit' between the simulation results and the 'known' or observed conditions of the system. Groundwater flow models are typically calibrated to head measurements at selected Observation Points, while contaminant transport models are typically calibrated to concentration measurements at selected Observation Points.

To display a Calibration Residual Map for the flow model, press the **[F9 - Overlay]** button in the toolbar along the bottom of the screen and select the **Cal - Head Residual - Values** option.

To display a Calibration Residual Map for the mass transport model, press the **[F9 - Overlay]** button in the toolbar along the bottom of the screen and select the **Cal - Conc. Residual - Values** option.

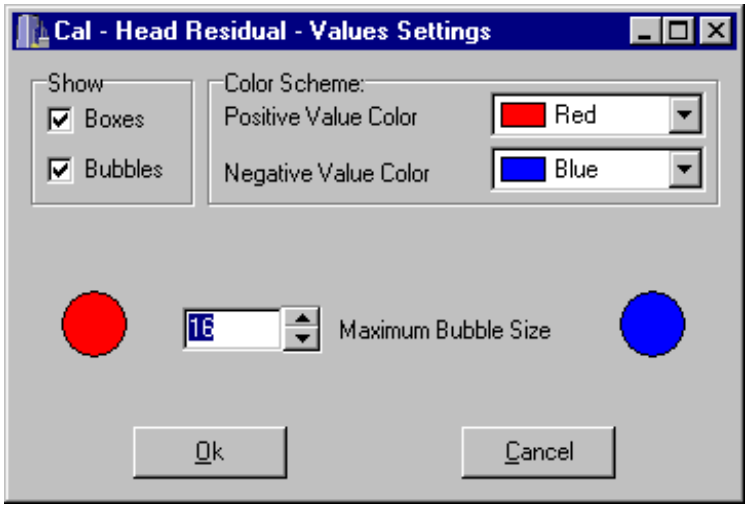
The Calibration Residual Map displays the observed and calculated values of Head and/or Concentration at selected Observation Points on the map, and displays a bubble plot of the Calibration Residuals at selected Observation Points on the map (see following figure). The size and color of the bubbles are scaled according to the Calibration Residual value at each Observation Point.

> **Note:** The Calibration Residual Map data will be displayed only for selected Observation Wells containing an Observation Point in the layer currently being viewed. For transient simulations, it is also important to note that the Calibration Residuals are plotted for the simulation time steps and NOT the actual observation times (i.e. the observed values are interpolated to the model time steps).



Calibration Residual Display Options

The display settings of the Calibration Residual Map can be modified by selecting the associated Browse button under the **Settings** column of the **Overlay Control** window. The Calibration Residual display settings window will appear as shown in the following figure and described below.



- The **Show** options control the information displayed on the Calibration Residual Map. The **Boxes**switch shows/hides the text boxes containing the calculated and observed values, and the **Bubbles** switch shows/hides the Calibration Residual bubbles.
- The **Color Scheme** options control the color of the Calibration Residual bubbles. Positive value Calibration Residual bubbles will be plotted using the **Positive Value Color**, while negative value Calibration Residual bubbles will be plotted using the **Negative Value Color**.
- The **Maximum Bubble Size** is used to set the size of the bubble corresponding to the maximum Calibration Residual value. All other bubble sizes will be scaled accordingly.

The Calibration Residual bubble plots are very helpful for quickly identifying regions of the model where the calibration is weakest and determining whether the model is over-predicting or under-predicting the observed values.

5.3 Graphs

Visual MODFLOW displays four different types of graphs:

- **Calibration** graphs
- **Time-Series** graphs
- **Mass Balance** graphs
- **Zone Budget** graphs

Each of these graph types and the associated display options are presented in the following sections

5.3.1 Calibration Graphs

Model calibration is the process whereby selected model input parameters are adjusted within reasonable limits to produce simulation results that best match the known or measured values. Model calibration is the most critical process in building the groundwater flow and contaminant transport model, because the quality of the calibration inevitably determines the reliability of any conclusions and recommendations made using the simulation results.

The acceptability of a model's calibration is usually a subjective measure because each model has different objectives and must be calibrated to different conditions. However, there are some generally accepted methods of evaluating and interpreting the model calibration using both qualitative and quantitative measures.

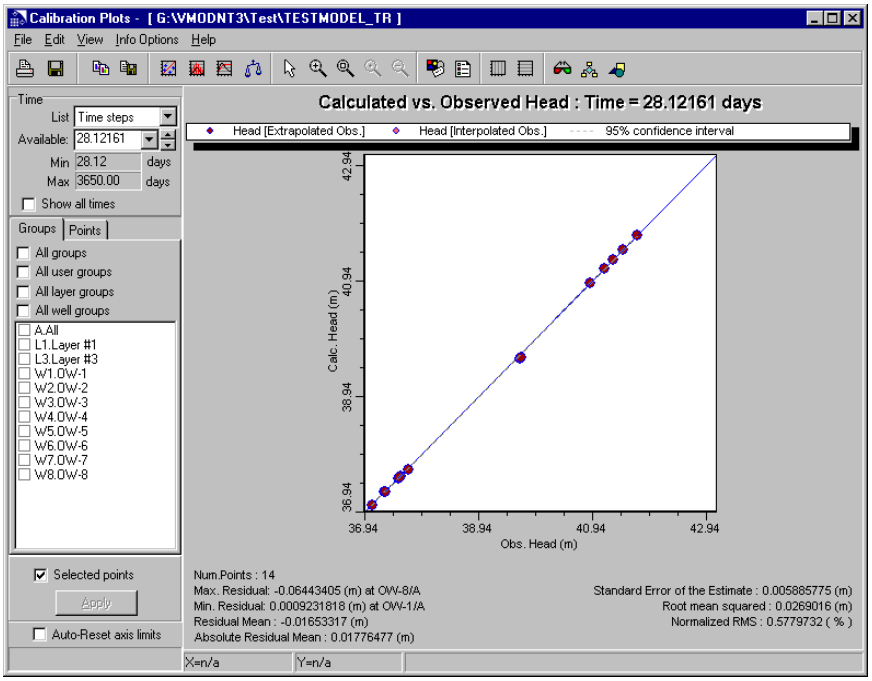
Visual MODFLOW provides a comprehensive selection of model calibration analysis tools for evaluating, interpreting and presenting the model calibration including:

- Calculated vs. Observed Scatter Graph

- Calibration Residuals Histogram
- Calculated and Observed Values vs. Time
- Calibration Statistics vs. Time

Calibration Graphs may be displayed in the **Output** section by selecting **Graphs/ Calibration** from the top menu bar and choosing either **Head** or **Concentration**. The default Calibration Graph is a scatter plot of Calculated vs. Observed values for the selected Observation Wells as shown in the following figure.

The **Calibration Plots** window is the 'Command Centre' for the four different types of Calibration Graphs. Each of the Calibration Graphs are plotted using the IChart graphing component described in Chapter 6. The following sections described the specific features and functionality of the Calibration Graphs not covered in Chapter 6.



When the **Calibration Plots** window is first opened, it will display a Calculated vs. Observed Scatter Graph of the Observation Points selected in the Visual MODFLOW screen (see section Selecting Observation Points on page 233). However, the **View** options on the top menu bar may be used to selected either of the four types of Calibration Graphs. Alternatively, the following **Calibration Plots** toolbar icons may also be used to switch between the different calibration graphs.

[Calc. vs Obs.] Plots the Calculated vs. Observed Scatter Graph. For details please refer to section Calculated vs. Observed Scatter Graphs on page 248.

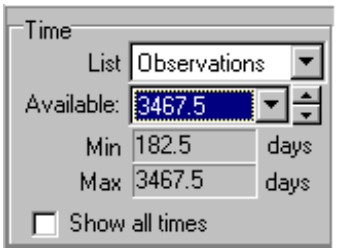
	[Residual Distribution]	Plots the Calibration Residual Distribution Histogram. For details please refer to section Calibration Residuals Histogram on page 251.
	[Head vs. Time]	Plots the Head (or Concentration) versus Time graph. For details please refer to section Head or Concentration vs. Time Graphs on page 252.
	[Statistics vs. Time]	Plots Calibration Statistics vs. Time. For details please refer to section Calibration Statistics vs. Time Graphs on page 253.

Calibration Times

The Calculated vs. Observed Scatter Graph and the Calibration Residuals Histogram represents a snap-shot in time of the comparison between the calculated and observed values. For transient simulations containing many different observation times for each observation point, the quality of the model calibration will likely change throughout the simulation. Therefore, it is important to be able to evaluate the calibration at different times throughout the simulation.

Unfortunately, the output times generated by MODFLOW rarely coincide with the actual times when the observed data was collected or recorded in the field. However, it is generally considered a good practice to interpolate the model calculated data to the observation times in order to compare the calculated vs. observed values.

The **List** field contains a selection of four different lists of Output times to compare and plot the Calculated vs. Observed data.



- The **Time Steps** list contains the times from each model time step
- The **Observations** list contains a merged compilation of the observation times from all Observation Points
- The **Stress Periods** list contains the time from the end of each Stress Period
- The **Output Times** list contains the model **Output Control** times

Once the **Time List** is selected, the corresponding list of times will be available to choose from the **Available** field, and the minimum and maximum time values will be shown in the **Min.** and **Max.** fields, respectively.

As mentioned above, it is recommended to choose the **Observations List** in order to compare the calculated values vs. the observed values at the actual observation times.

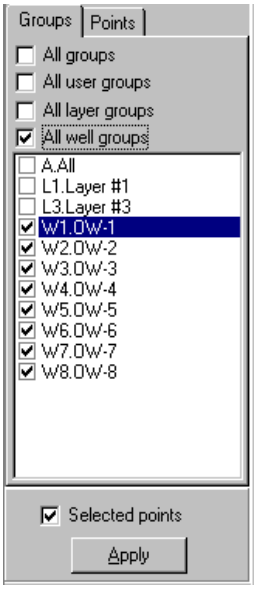
The **Show all times** option shows the calculated vs. observed data for all output times. This is a valuable feature to see how the calibration patterns change with time.

Observation Points

When the **Calibration Plots** window is first opened it will display the Calculated vs. Observed Scatter Graph for the selected Observation Points (see section Selecting Observation Points on page 233). However, the Observation Points displayed on the graph can be modified on-the-fly by activating or de-activating selected Observation Groups or individual Observation Points.

The **Groups** tab provides a listing of the available Observation Groups:

- **A.All** displays all Observation Points.
- **L1.Layer #*N*** displays Observation Points in the selected Layer Group.
- **U1.*Name*** displays Observation Points in the selected User-Defined Group.
- **W1.*Wellname*** displays Observation Points in the selected Well Group.



The **Points** tab provides a listing of the individual Observation Points.

Once the desired Observation Groups and/or Observation Points are selected, press the **[Apply]** button to update the Time Series Graph.

Chemical Species

For mass transport simulations involving multiple chemical species, an additional tab labelled **Species** will appear beside the **Group** and **Points** tabs. The **Species** tab contains a list of the Chemical Species being simulated by the model. One or more of these species can be selected to plot on the Time-Series Graph.

Once the desired Chemical Species are selected, press the [Apply] button to update the Time-Series Graph.

Info Options

Specific information about a data point on a graph may be obtained by simply clicking on the data point to display an Info bubble. The **Info Options** item in the top menu bar of the Calibration Plots window controls the information displayed for each data point on the graph and the format used to display the information.

Display Settings

The Time-Series Graphs are plotted using the IChart graphing component described in Chapter 6. Please refer to this chapter for a detailed description of the display settings available for customizing the appearance of the graph and for instructions on preparing and printing the graph.

Calculated vs. Observed Scatter Graphs

The Scatter Graph of Calculated vs. Observed Values is the default Calibration Graph. This graph represents a snap-shot in time of the comparison between the values calculated by the model (Y-axis) and the values observed or measured in the field (X-axis). In the example shown above, all of the data points intersect the 45 degree line on the graph where X=Y. This represents an ideal calibration scenario, but it's not likely to happen in many real-life circumstances.

If the data points appear above the X=Y line, then the calculated values are larger than the observed values and the Calibration Residual is positive and the model is over-predicting. If the data points are under the X=Y line then the calculated values are less than the observed values then the Calibration Residuals are negative and the model is under-predicting.

Interpolated and Extrapolated Data Points

As mentioned above, the output times from the model will rarely coincide with the actual observation times when data was measured in the field. As a result, the calculated data must be interpolated to the observation times in order to calculate the Calibration Residual for a specific snap-shot in time (or vice-versa).

- **[Interpolated Calc.]** data points represent calculated values at observation times where the observation time is between two model output times.
- **[Extrapolated Calc.]** data points represent calculated values at observation times where the observation time is outside the range of model output times.
- **[Interpolated Obs.]** data points represent observed values at model output times where the output time is between two observation times.
- **[Extrapolated Obs.]** data points represent observed values at model output times where the output time is outside the range of observation times.

95% Confidence Interval

The 95% Confidence Interval allows the user to visualize a range of calculated values for each observed value. Within this interval, the user can be 95 percent confident that the simulation results will be acceptable for a given observed value. The 95% Confidence Interval is calculated using the following equation:

$$Range = \pm 1.96 \cdot \sqrt{\frac{\sum (X_{obs} - X_{calc})^2}{n-2}} \cdot \sqrt{\frac{1}{n} + \frac{(X_{obs} - X_{avgobs})^2}{\sum X_{obs}{}^2 - \left(\frac{1}{n}\right)(\sum X_{obs})^2} + 1}$$

Where X_{obs} is the observed value, X_{calc} is the calculated value, X_{avgobs} is the average observed value, and n is the number of observations.

Calibration Statistics

In the footer of the Calculated vs. Observed Scatter Graph are listed several calibration statistics as described below.

Calibration Residual

The Calibration Residual is defined as the difference between the calculated results and the observed results as shown in the following equation:

$$R = \frac{1}{n} \sum_{i=1}^{n} (X_{calc} - X_{obs})_i$$

Where R is the Residual, X_{obs}. is the observed value and X_{calc}. is the calculated value for a data series.

Number of Residuals

The number of Residuals (n) is the total number of observations selected for a particular "snapshot" in time. For example, if you select L1.Layer#1 and there are 10 wells in the Layer#1 group, then the Number of Residuals is 10.

Residual Mean

The Residual Mean is a measure of the average Residual value defined by the equation:

$$\bar{R} = \frac{1}{n} \sum_{i=1}^{n} R_i$$

Note that there may be cases where over-calculated and under-calculated values will negate each other and produce a Residual Mean value close to zero. This can lead to false interpretation of the model calibration. The Residual Mean should never be used by itself as a measure of the fit between the simulated results and the observed data.

Absolute Residual Mean

The Absolute Residual Mean is similar to the Residual Mean except that it is a measure of the average absolute Residual value defined by the equation:

$$|\bar{R}| = \frac{1}{n} \sum_{i=1}^{n} |R_i|$$

The Absolute Residual Mean measures the average magnitude of the Residuals and therefore provides a better indication of calibration than the Residual Mean.

Standard Error of the Estimate

The Standard Error of the Estimate (SEE) is a measure of the standard deviation of the estimate and is expressed by the equation:

$$SEE = \sqrt{\frac{\frac{1}{n-1}\sum_{i=1}^{n}(R_i - \bar{R})^2}{n}}$$

Root Mean Squared Residual

The root mean squared error (RMS) is defined by the equation:

$$RMS = \frac{1}{n}\sqrt{\sum_{i=1}^{n} R_i^2}$$

Normalized Root Mean Squared Residual

The Normalized Root Mean Squared Residual is the RMS divided by the maximum difference in the observed head values and is expressed by the equation:

$$NormalizedRMS = \frac{RMS}{(X_{obs})_{max} - (X_{obs})_{min}}$$

The Normalized RMS is expressed as a percentage and is a more representative measure of the fit than the standard RMS because it accounts for the scale of the potential range of data values.

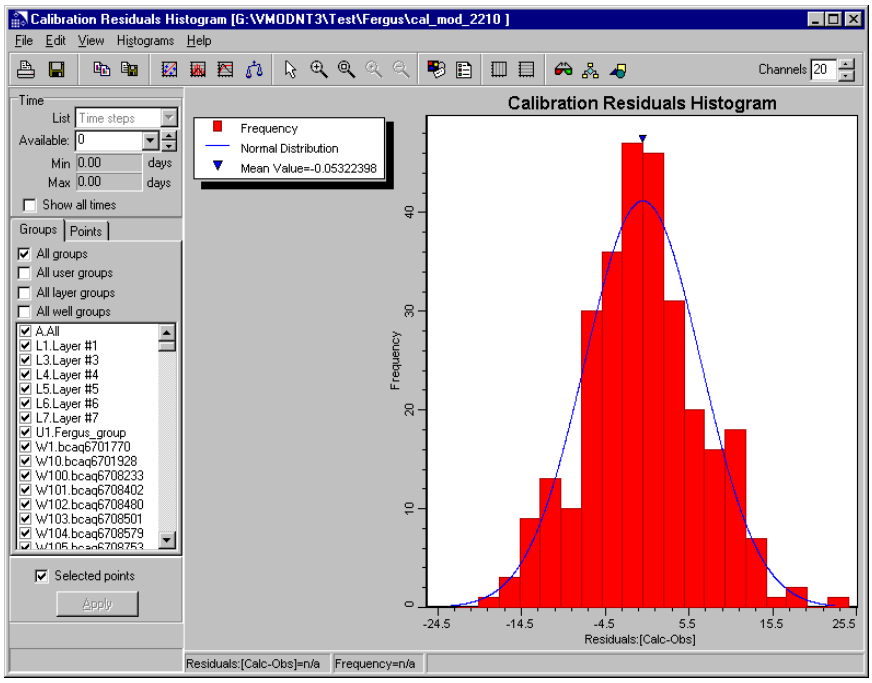
For example, an RMS value of 1.5 will indicate a poor calibration for a model with a range of observed values between 10 and 20, but it will indicate an excellent calibration for a model with a range of observed values between 100 and 200. However, the Normalized RMS value for the first model would be 15%, while the Normalized RMS for the second model would be 1.5%. In this situation, the Normalized RMS values clearly indicates the second model provides a good fit between the calculated and observed values.

Calibration Residuals Histogram

To display a Calibration Residuals Histogram:

- Select **Graphs/Calibration** from the top menu bar of the **Output** section and choose either **Head** or **Concentration**.
- A **Calibration Plots** window will appear with a Calculated vs. Observed Scatter Graph.
- Select **View/Residual Distribution** from the top menu bar of the **Calibration Plots** window to switch to the Calibration Residuals Histogram.

The Calibration Residuals Histogram displays the Population, Frequency, or Relative Frequency of observations for specified intervals of the Normalized Calibration Residual values. The Normalized Calibration Residual values are calculated using the above mentioned formulas for each data series.



The number of groups of observation points or channels is specified in the top menu bar using the **Channels** property box. The default number of **Channels** is 20. This value can be increased or decreased using the up and down arrow buttons.

The Normal Distribution curve is a two-tailed p-value of a Z-test. This curve can be used to determine the likelihood an observation lies in a particular population.

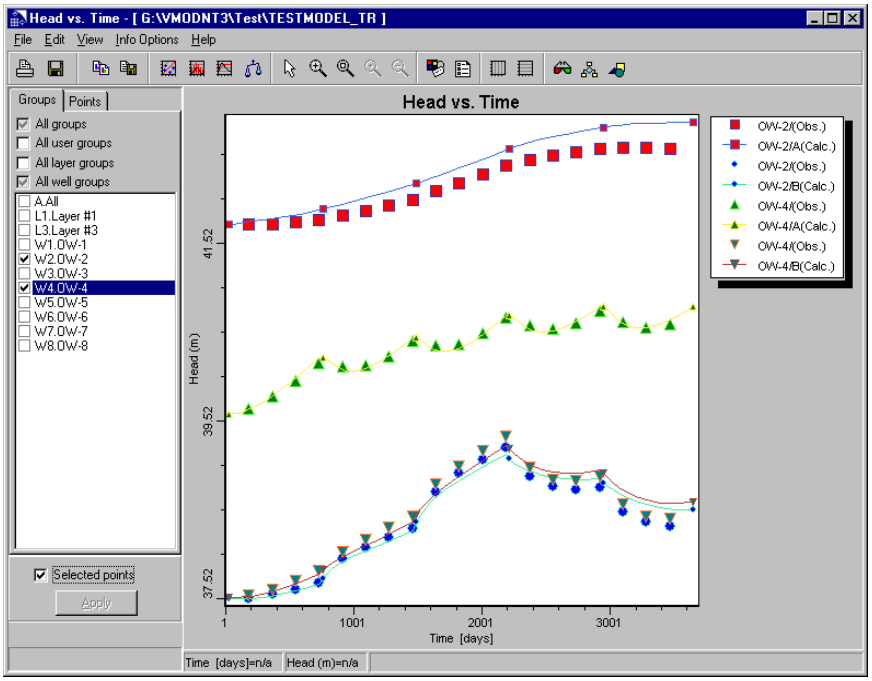
The Residual Distribution Histogram provides a qualitative comparison of the distribution of the normalized calibration residual values against the student distribution curve. Ideally, the distribution of the calibration residuals for a large

number of observation points would be similar to that of the student distribution curve, with most of the residuals groups clustered around the value of zero.

Head or Concentration vs. Time Graphs

To display a Time-Series Graph of Head or Concentration:

- Select **Graphs/Calibration** from the top menu bar of the **Output** section and choose either **Head** or **Concentration**.
- A **Calibration Plots** window will appear with a Calculated vs. Observed Scatter Graph.
- Select **View/Head vs. Time** from the top menu bar of the **Calibration Plots** window to switch to the Time-Series Graph of Head or Concentration.



This graph displays a time series plot of observed and calculated values for each selected Observation Point. If the time series plot appears with only one data point for each Observation Point then the simulation was likely run for Steady-State conditions and a time-series graph is not relevant, or the transient simulation is set to print the results only at the end of the simulation.

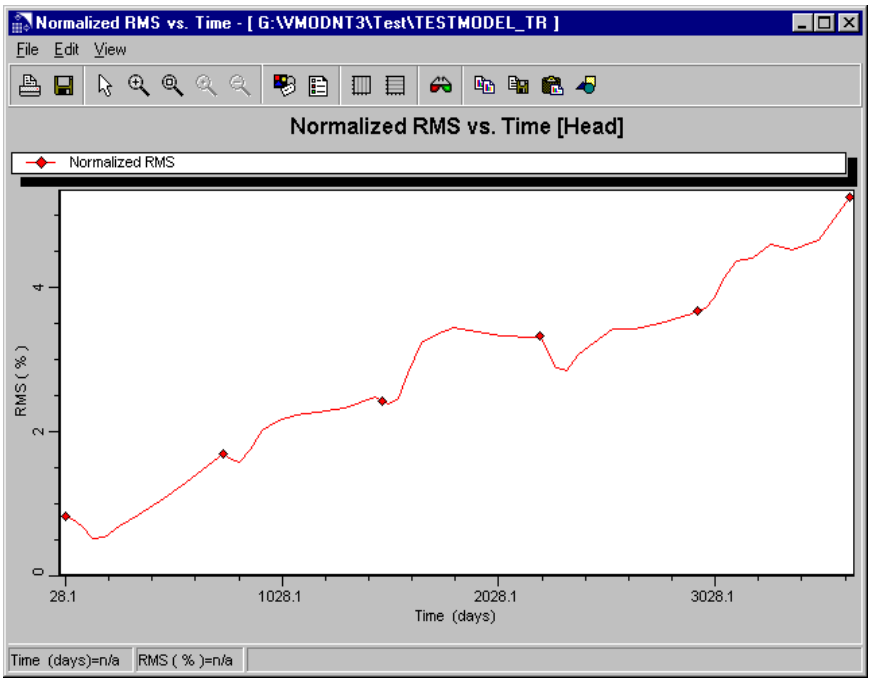
If more than twenty Observation Points are selected, a message will appear warning that it may take a while to process all of the data and the resultant graph will likely be too cluttered to make much sense out of.

The ability to plot time series graphs for selected observation points allows the user to calibrate the model to both steady-state and transient conditions, ensuring the uniqueness of the model solution and the reliability of the results.

Calibration Statistics vs. Time Graphs

To display a Time-Series Graph of Calibration Statistics:

- Select **Graphs/Calibration** from the top menu bar of the **Output** section and choose either **Head** or **Concentration**.
- A **Calibration Plots** window will appear with a Calculated vs. Observed Scatter Graph.
- Select **View/Statistics vs. Time** from the top menu bar of the **Calibration Plots** window to switch to the Time-Series Graph of Calibration Statistics.



The Calibration Statistics vs. Time Graph displays the various statistical measures of the model calibration throughout the entire simulation. The available calibration statistics include:

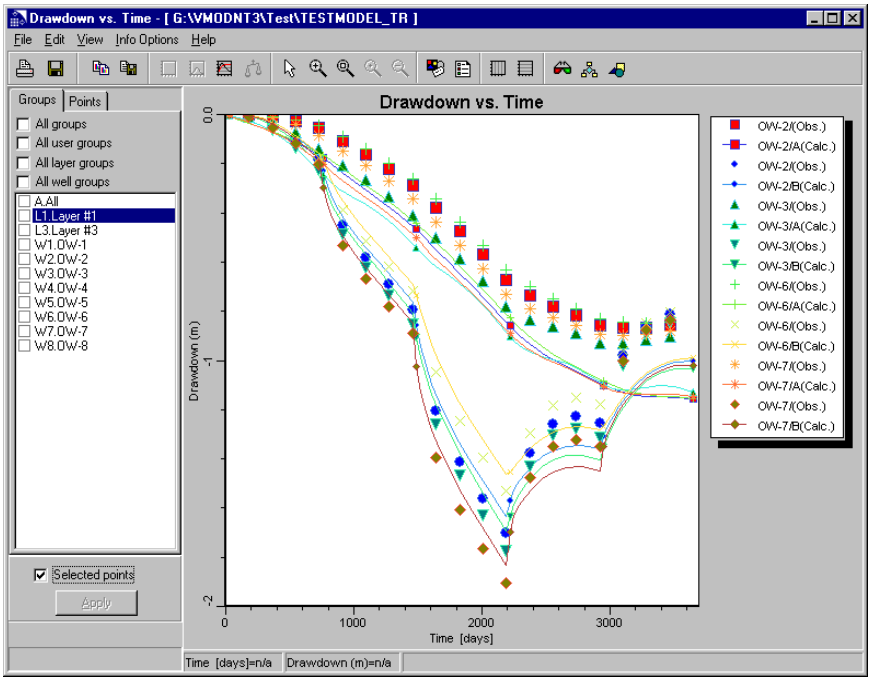
- **Normalized RMS**
- **Residuals**
- **Normalized Residuals**
- **Errors**

These different graphs can be displayed by selecting the desired graph type from the **View** item in the top menu bar.

In the graph shown above the Normalized RMS is increasing with time, indicating the quality of the model calibration is deteriorating towards the end of the simulation.

5.3.2 Time-Series Graphs

A time-series graph plots the change in a selected variable(s) with time. In groundwater flow and contaminant transport modeling, time-series graphs are used to evaluate and compare temporal trends in the calculated Head, Drawdown, and Concentration at selected Observation Points. To plot a Time-Series Graph in Visual MODFLOW, select **Graph/Time-Series** from the top menu bar of the **Output** section and choose either **Head**, **Drawdown** or **Concentration**. A Time-Series Graph window will appear plotting both the calculated and observed values for the selected Observation Points as shown in the following figure (for information on selecting Observation Points please refer to section Selecting Observation Points on page 233).

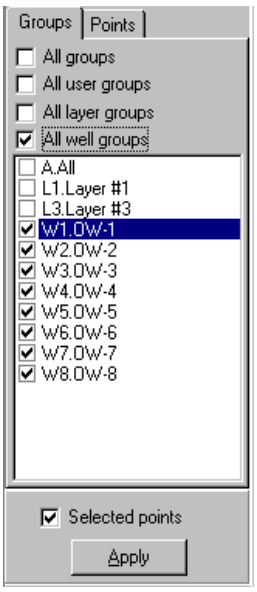


The above figure displays a Drawdown vs. Time Graph for eight different Observation Points selected in the main Visual MODFLOW screen. By default, each Observation Point will be plotted using different symbols, and the calculated and the observed values for each Observation Point are differentiated by the symbol size, whereby the symbol for the Observed data series is larger than the symbol for the calculated data series. In addition, the data series for the calculated values is plotted using lines to join

each data point, whereas the data series for the observed values is plotted using only a symbol at each data point.

If no observation data is present, then only the calculated values will appear.

Observation Points



When the Time Series Graph is first opened it will display data for the selected Observation Points (see section Selecting Observation Points on page 233). However, the Observation Points displayed on the graph can be modified on-the-fly by activating or de-activating Observation Groups or individual Observation Points using the **Groups** and **Points** tabs, respectively.

The **Groups** tab provides a listing of the available Observation Groups:

- **A.All** displays all Observation Points.
- **L*N*.Layer #*N*** displays Observation Points in the selected Layer Group.
- ***UN.Name*** displays Observation Points in the selected User-Defined Group.
- **W*N.Wellname*** displays Observation Points in the selected Well Group.

The **Points** tab provides a listing of the individual Observation Points.

Once the desired Observation Groups and/or Observation Points are selected, press the **[Apply]** button to update the Time Series Graph.

Chemical Species

For mass transport simulations involving multiple chemical species, an additional tab labelled **Species** will appear beside the **Group** and **Points** tabs. The **Species** tab contains a list of the Chemical Species being simulated by the model. One or more of these species can be selected to plot on the Time-Series Graph.

Once the desired Chemical Species are selected, press the [Apply] button to update the Time-Series Graph.

Info Options

Specific information about a data point on a graph may be obtained by simply clicking on the data point to display an Info bubble. The **Info Options** item in the top menu bar of the Calibration Plots window controls the information displayed for each data point on the graph and the format used to display the information.

Display Settings

The Time-Series Graphs are plotted using the IChart graphing component described in Chapter 6. Please refer to this chapter for a detailed description of the display settings available for customizing the appearance of the graph and for instructions on preparing and printing the graph.

5.3.3 Mass Balance Graphs

The finite difference formulation of both the groundwater flow equation and the mass transport equation is based on conservation of mass such that the mass of water or chemicals entering the system through various sources should equal the mass of water or chemicals leaving the system through the various sinks. The Mass Balance Graphs provide graphical representations of the mass of water or chemicals entering and leaving the system through the various sources and sinks.

Flow Mass Balance Graphs

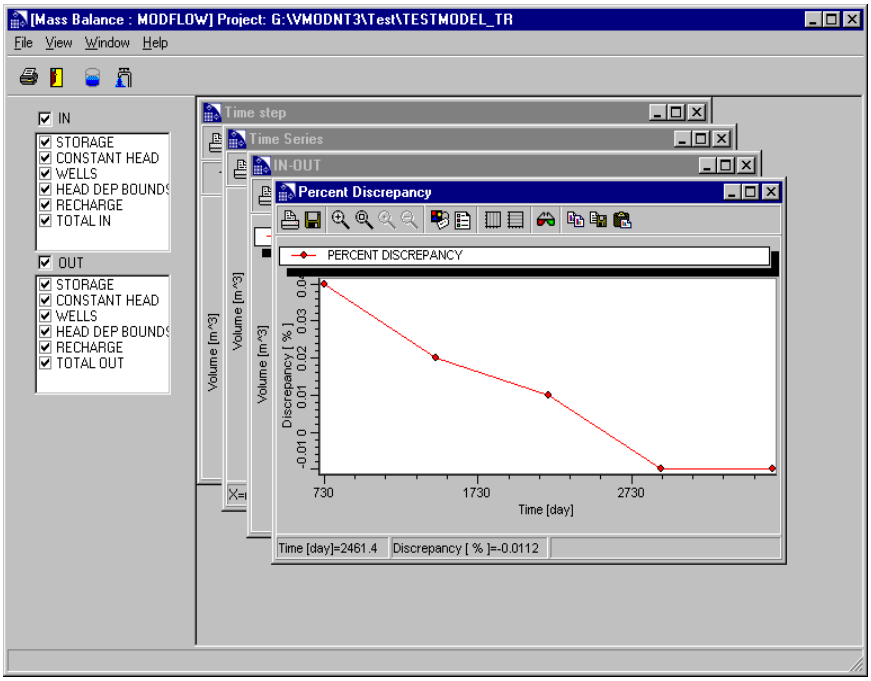
The Flow Mass Balance Graphs plot the volume and rates of water entering and leaving the system through the flow boundary conditions and from aquifer storage at each Output Time.

To plot the Flow Mass Balance Graphs select **Graphs/Mass Balance/Flow** from the top menu bar of the **Output** section and a **Mass Balance: MODFLOW** window will appear as shown in the following figure.

There are four different Flow Mass Balance Graphs:

- **Percent Discrepancy** plots the temporal changes in the Flow Mass Balance (total flow IN minus total flow OUT) expressed as a percentage of the total flow.
- **IN - OUT** plots the temporal change in the Flow Mass Balance (total flow IN minus the total flow OUT).
- **Time Series** plots the temporal flows IN and OUT of the system through the individual sources and sinks (flow boundary conditions and storage).
- **Time Steps** plots a bar chart of the flow IN to the system and the flow OUT of the system through the individual sources and sinks (flow boundary conditions and storage) for selected Output Times.

As mentioned above, the Flow Mass Balance Graphs can be used to plot the flow volume or flow rates of water coming IN and going OUT of the system. By default, the **Mass Balance: MODFLOW** window plots the flow volume mass balance. Use the **View** option in the top menu bar to select either **Volume** or **Rates**, or click the **[Cumulative volume]** or **[Rate]** icon in the toolbar.



Sources and Sinks

On the left-hand side of the **Mass Balance: MODFLOW** window is a list of all potential sources and sinks for the current flow model (boundary conditions not included in the model will not be listed). These sources and sinks are included in both the **IN** list and the **OUT** list. The **IN** list contains a summary of the flow coming into the system from each individual source term, while the **OUT** list contains a summary of the flow going out of the system through each individual sink term.

These controls can be used to add or remove the individual source and sink terms from either the **Time Series** graph or the **Time Steps** graph.

The **Percent Discrepancy** graph and the **IN-OUT** graph consider only the total flow in to and out of the entire system as a whole. As a result, the settings for the individual **IN** and **OUT** terms do not influence the results and appearance of these graphs.

Arranging the Graphs

Each of the Flow Mass Balance Graphs can be maximized to occupy the entire **Mass Balance** window by clicking maximize button in the top right-hand corner of each graph window.

Alternatively, the graphs can be tiled in the **Mass Balance** window by selecting **Windows/Tile** from the top menu bar.

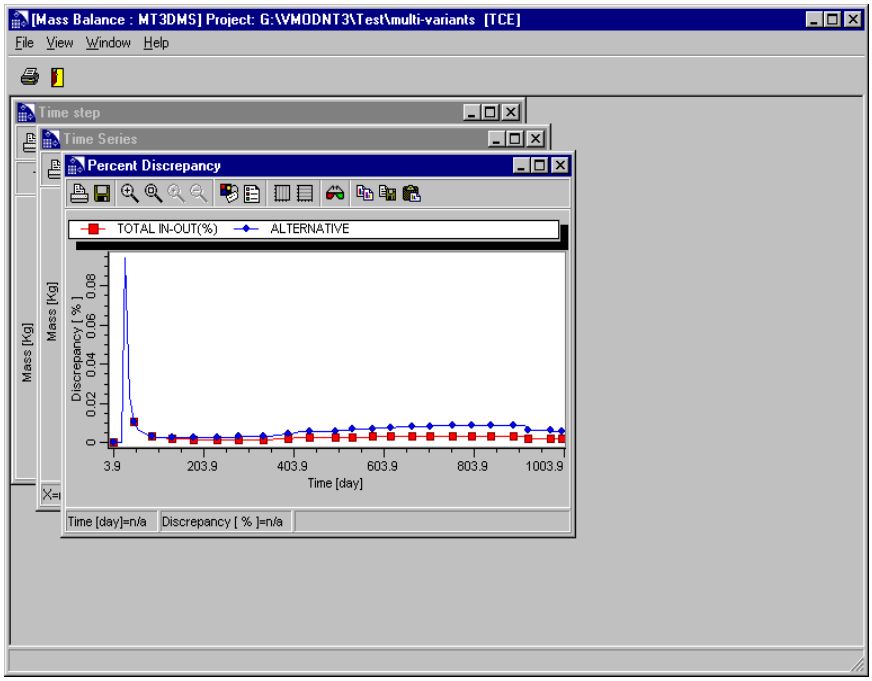
Customizing and Printing the Graphs

The Flow Mass Balance Graphs are all plotted using the IChart graphing component described in Chapter 6. Please refer to this chapter for a detailed description of the display settings available for customizing the appearance of the graphs and for instructions on preparing and printing the graphs.

Transport Mass Balance Graphs

The **Transport** Mass Balance Graphs plot the mass of chemicals entering and leaving the system through all sources and all sinks, and the total mass of chemicals remaining in the system at each Output Time.

To plot the Transport Mass Balance Graphs select **Graphs/Mass Balance/Flow** from the top menu bar of the **Output** section and a **Mass Balance: MT3D** window will appear as shown in the following figure.



By default, the Transport Mass Balance Graphs will be plotted for the current chemical species in the **Concentration Contour Map** screen. If the **Concentration Contour Map** is not being displayed, the Transport Mass Balance Graphs will be plotted for the first chemical species in the list. To plot the Transport Mass Balance Graphs for a different chemical species, open the **Concentration Contour Map** and use the **[Species]** button to select a new Chemical Species.

There are three different Transport Mass Balance Graphs:

- **Percent Discrepancy** plots the temporal changes in the Transport Mass Balance (cumulative mass IN minus cumulative mass OUT) expressed as a percentage of the cumulative mass IN.
- **Time Series** plots the temporal changes in the cumulative mass entering, remaining and leaving the system (where; SOURCE IN is the mass entering through sources; SINKS OUT is the mass leaving the system through sinks; TOTAL MASS IN AQUIFER is the mass remaining; TOTAL IN is the mass added to the system through changes in the mass storage; and TOTAL OUT is mass removed from the system through changes in the mass storage).
- **Time Steps** plots a bar chart of the cumulative mass that has entered, remains and has left the system at a specified Output Time.

With both the Time Steps and the Time Series graph it is important to remember that this graph presents the cumulative mass at a point in time, and not the mass loading rate at this point in time. In addition, when interpreting these graphs it is important to remember that the TOTAL IN and TOTAL OUT value do NOT represent mass entering or leaving the system through external sources and sinks, but rather it is a reflection of the mass being internally 'moved' from one grid location to another (i.e. mass is moved OUT of one cell and IN to another).

Arranging the Graphs

Each of the Transport Mass Balance Graphs can be maximized to occupy the entire Mass Balance window by clicking maximize button in the top right-hand corner of each graph window.

Alternatively, the graphs can be tiled in the Mass Balance window by selecting **Windows/Tile** from the top menu bar.

Customizing and Printing the Graphs

The Transport Mass Balance Graphs are all plotted using the IChart graphing component described in Chapter 6. Please refer to this chapter for a detailed description of the display options available for customizing the appearance of the graphs and for instructions on preparing and printing the graphs.

5.3.4 Zone Budget Graphs

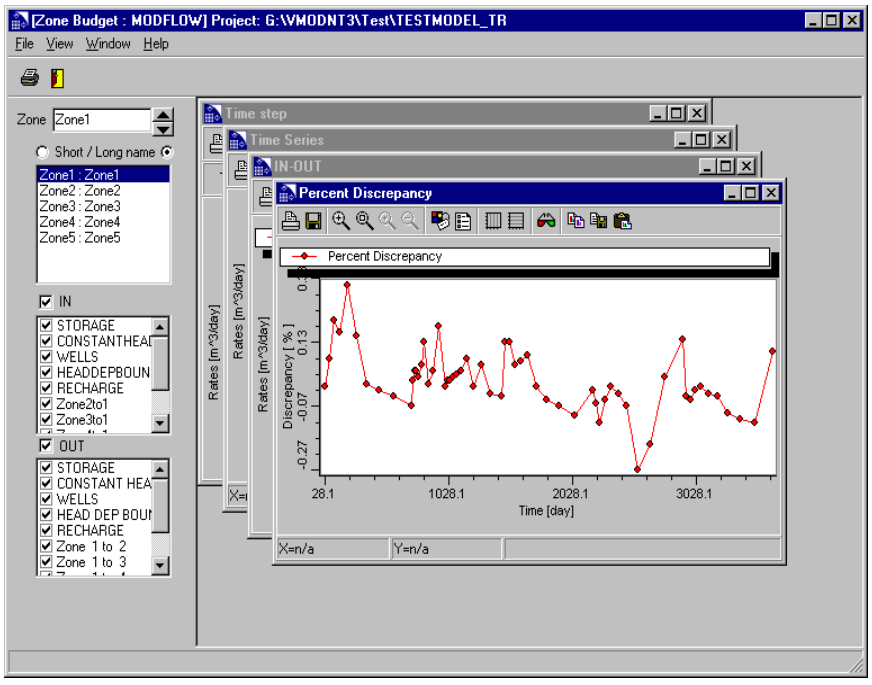
Zone Budget is a program developed by the U.S. Geological Survey to calculate water budgets for user-defined zones in the model. The user-defined Zone Budget zones are defined in the **Input** section in the **ZBud** screen (see section Zone Budget on page 152). The Zone Budget program essentially calculates the flow mass balance (see section Flow Mass Balance Graphs on page 256) for each user-defined zone.

For mass transport simulation, the transport mass balance (see section Transport Mass Balance Graphs on page 258) can also be calculated for the same user-defined zones if MT3D96 or MT3D99 are being used.

Flow Zone Budget Graphs

The Flow Zone Budget Graphs plot the flow rates of water entering and leaving the user-defined zones through the flow boundary conditions, from aquifer storage, and through other user-defined zones.

To display the Flow Zone Budget Graphs select **Graphs/Zone Budget/Flow** from the top menu bar of the **Output** section and a **Zone Budget: MODFLOW** window will appear as shown in the following figure.

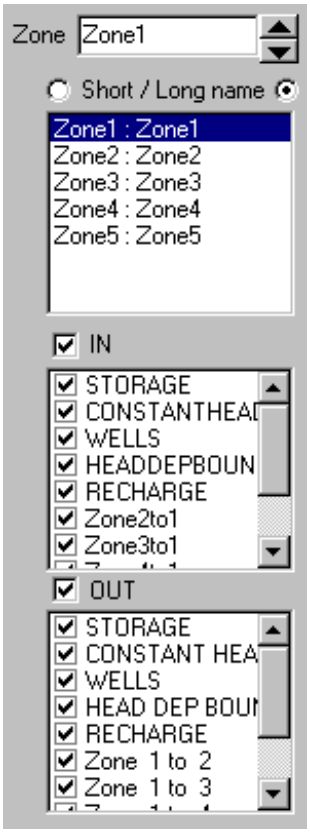


There are four different Flow Zone Budget Graphs:

- **Percent Discrepancy** plots the temporal changes in the Flow Mass Balance for the selected zone (total flow IN minus total flow OUT) expressed as a percentage of the total flow in the zone.
- **IN - OUT** plots the temporal change in the Flow Mass Balance for the selected zone (total flow IN minus the total flow OUT).
- **Time Series** plots the temporal flows IN and OUT of the selected zone through the individual sources and sinks (flow boundary conditions and storage).
- **Time Steps** plots a bar chart of the flow IN to the system and the flow OUT of the selected zone through the individual sources and sinks (flow boundary conditions and storage) for selected Output Times.

Selecting Zones

On the left-hand side of the **Zone Budget: MODFLOW** window is a list of the Zone Budget zones available for the current model. The Zone Budget graphs described above will display the Zone Budget data for the selected Zone Budget zone.



Sources and Sinks

The IN list contains each of the possible source terms which may contribute flow to the selected Zone Budget zone, while the OUT list contains each of the possible sink terms which may divert flow out of the selected Zone Budget zone.

The checkboxes beside each term can be used to add or remove the individual source and sink terms from either the **Time Series** graph or the **Time Steps** graph.

The **Percent Discrepancy** graph and the **IN-OUT** graph consider only the total flow in to and out of the entire system as a whole. As a result, the settings for the individual **IN** and **OUT** terms do not influence the results and appearance of these graphs.

Arranging the Graphs

Each of the Flow Mass Balance Graphs can be maximized to occupy the entire **Zone Budget** window by clicking maximize button in the top right-hand corner of each graph window.

Alternatively, the graphs can be tiled in the **Zone Budget** window by selecting **Windows/Tile** from the top menu bar.

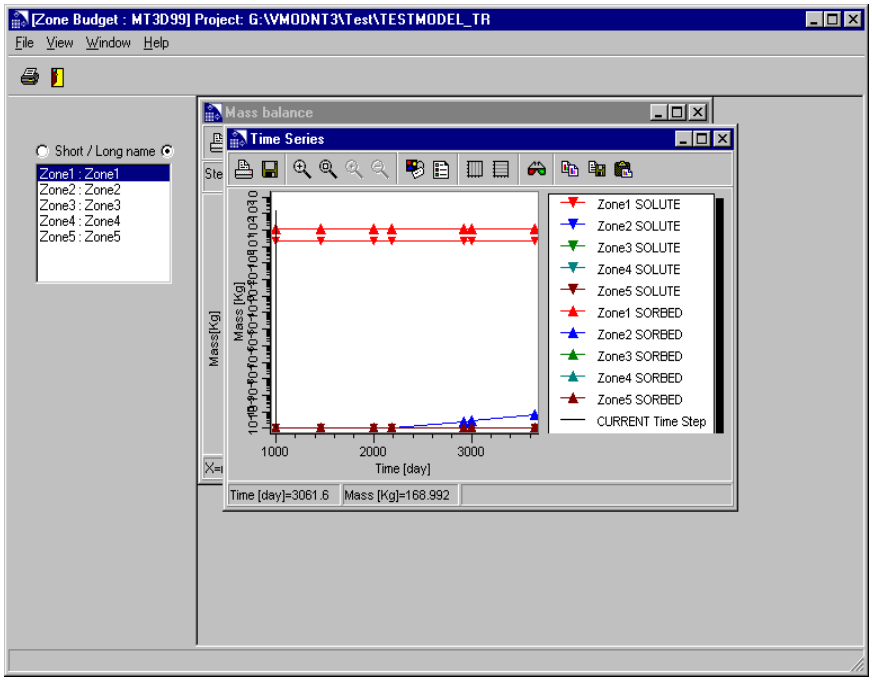
Customizing and Printing the Graphs

The Zone Budget Graphs are all plotted using the IChart graphing component described in Chapter 6. Please refer to this chapter for a detailed description of the display settings available for customizing the appearance of the graphs and for instructions on preparing and printing the graphs.

Transport Mass Balance Graphs

The **Transport** Zone Budget Graphs plot the dissolved and sorbed phase chemical mass in each Zone Budget zone at each Output Time.

To plot the Transport Mass Balance Graphs select **Graphs/Mass Balance/Flow** from the top menu bar of the **Output** section and a **Mass Balance: MT3D** window will appear as shown in the following figure.



By default, the Transport Zone Budget Graphs will be plotted for the current chemical species in the **Concentration Contour Map** screen. If the **Concentration Contour Map** is not being displayed, the Transport Zone Budget Graphs will be plotted for the first chemical in the species list. To select a different chemical species, open the **Concentration Contour Map** and use the **[Species]** button to select a new Chemical Species.

There are two different Transport Zone Budget Graphs:

Time Series	Plots the cumulative chemical mass dissolved (SOLUTE) and sorbed (SORBED) in each Zone Budget zone.
Time Steps	Plots a bar chart of the cumulative mass dissolved (SOLUTE) and sorbed (SORBED) in each Zone Budget zone for selected Output Times.

With both the **Time Steps** and the **Time Series** graph it is important to remember that this graph presents the cumulative mass at a point in time, and not the mass loading rate at this point in time.

Arranging the Graphs

The Transport Zone Budget Graphs can be maximized to occupy the entire **Zone Budget** window by clicking maximize button in the top right-hand corner of each graph window.

Alternatively, the graphs can be tiled in the **Zone Budget** window by selecting **Windows/Tile** from the top menu bar.

Customizing and Printing the Graphs

The Transport Mass Balance Graphs are all plotted using the IChart graphing component described in Chapter 6. Please refer to this chapter for a detailed description of the display options available for customizing the appearance of the graphs and for instructions on preparing and printing the graphs.

5.4 Tools

The **Tools** menu item has the following options:

Cell Inspector	Displays the cell values for selected model parameters including grid co-ordinates, Kx, Ky, Kz, Ss, Sy, Head, and Concentration.
Annotate	Add lines, shapes, and text to the display screen.

5.4.1 Cell Inspector

The Cell Inspector is used to inspect selected model parameter values on a cell-by-cell basis using the mouse to select the grid cell of interest. A detailed description of the Cell Inspector and instruction on how to use it are provided in the section Cell Inspector on page 155.

5.4.2 Annotate

Some basic graphics features have been included in Visual MODFLOW to add text, lines, arrows, and shapes to the model display screen.

To add some basic graphics to the model display area, choose **Tools/Annotate** from the top menu of the Input section and the following options appear on the left-hand toolbar:

[Add] Add an **Arrow**, **Rectangle**, **Circle**, **Text** or **Line** to the current layer, row, or column.

[Erase] Erase a single graphic object or erase a group of object by stretching a box around the objects.

[Edit Single] Edit the properties associated with selected graphic objects.

[Move Single] Move selected graphic objects by clicking-and-dragging the object to a new location.

6

IChart - Graphing and Mapping Component

IChart is a charting and plotting component developed by Waterloo Hydrogeologic for the purpose of displaying and printing a variety of graph and map formats including:

- X-Y scatter graphs (multiple data series)
- Time-series graphs (multiple data series)
- Bar charts (multiple data series)
- Contour maps
- Color maps

The IChart component is used throughout Visual MODFLOW for displaying and presenting the plot types listed above. This chapter describes the features and functionality of IChart under the following topic headings:

- Toolbar Icons
- Graph Properties
    - •Axis Settings
    - •Titles Settings
    - •Series Settings
    - •Legend Settings
    - •General Settings
    - •Info Settings
- Map Properties
    - •Contour Settings
    - •Color Map Settings
- Annotation Tools
- Printing Options
- Exporting Data
- Saving to a Graphics File

Any of the “Settings” listed above may be accessed by right-clicking mouse anywhere on the display area of the graph.

6.1 Toolbar Icons

This sections describes the functionality of the toolbar icons available from the various IChart plots. The icons are described in the usual order or their appearance (from left to right) in the toolbar. Please note that the available icons are not the same for each type of plot being displayed, so some of the icons described below may not be available (or appropriate) for the current plot being displayed.

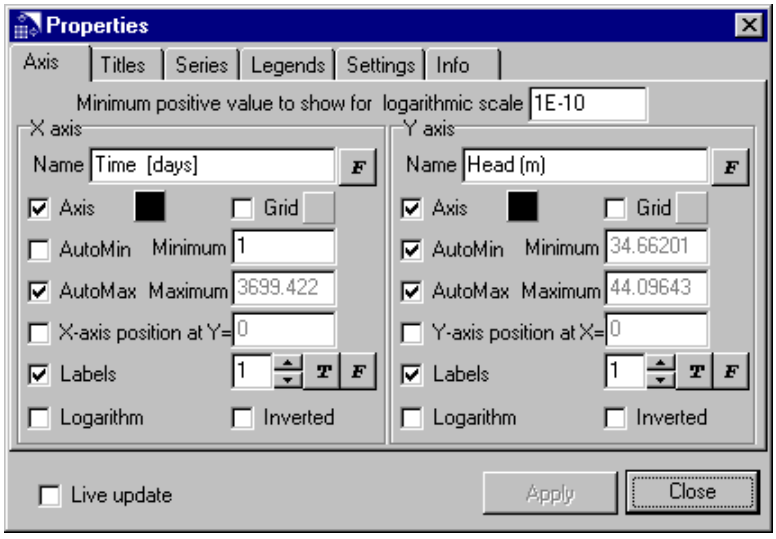
Print graphic	Opens the Print options window described on page 280.
Save As...	Saves plot to a graphics file (.BMP, .EMF or .WMF)
Copy to clipboard	Copies a bitmap image of the plot to the clipboard.
Export data	Exports selected data series to an ASCII text file as described on page 284
Pointer	Click on plot to display info for a selected data point or a selected location on the plot
Zoom in	Zoom in on a selected region of the plot.
Animated zoom	Animated zoom in to a selected location.
Zoom previous	Zoom out to the previous zoom setting
Zoom out	Zoom out to view the entire plot area.
Graph properties	Open the graph Properties window as described in the next section.
Show legend	Shows/hides the legend for the plot.
Vertical grid	Displays vertical grid lines at each major tick on X-axis
Horizontal grid	Displays horizontal grid lines at each major tick on Y-axis
3D view	Create 3D view of the graph axes and data series
Refresh	Refreshes the display of the graph

	Import data	Add a data series to the graph
	Paint	Add text, lines, shapes and arrows to the graph

6.2 Graph Properties

The appearance properties of the graph can be modified by right-clicking on the display area of the graph and choosing the Properties option, or by clicking the Graph properties icon from the toolbar.

The Properties window for the graph will appear as shown in the following figure.



The graph Properties window contains a series of tabs containing the appearance settings for the categories described in the following sections.

Save and Load Settings

Once the desired appearance properties for the graph are finalized, these settings may be saved for fast recall at a later time by selecting File/Save settings from the top menu bar. Once these settings are saved they can be quickly recalled next time by simply selecting File/Load settings from the top menu bar.

6.2.1 Axis Settings

The Axis settings tab (see figure above) controls the appearance of the X and Y axes on the graph, including the axis title, minimum and maximum axis values, tick mark labels and scale.

The Axis switch shows/hides the axis line, ticks and labels. The color box beside the Axis switch is used to select the color of the axis line.

The Grid switch hides/shows the grid lines for each tick along the axis. The color box beside the Grid switch is used to select the color of the grid lines.

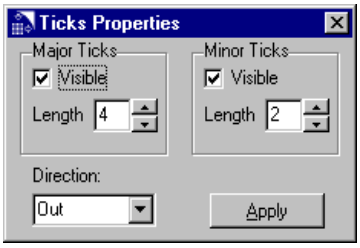
The Minimum positive value to show for logarithmic scale is used when switching either axis from a normal scale to a logarithmic scale. This value is used as a default minimum value for the axis if the normal scale minimum is negative or zero.

The Name field is the label for the axis. This value will be plotted under the X-axis and to the left of the Y-axis. The [***F***] button beside the Name field is used to select the font, size and color of the text.

The Automin and Automax options will automatically determine the minimum and maximum values, respectively, to plot on the axis. These value are displayed in the Minimum and Maximum fields. If the Automin and Automax fields are not selected, then user-defined Minimum and Maximum value may be entered.

The X-axis position at option defines the Y value where the X-axis will be plotted through the graph. The default setting is to plot the X-axis corresponding the Minimum value of the Y-axis.

The Labels option defines the frequency of tick labels. A value of 1 will label each major tick mark along the axis. A value of 2 will label every 2nd major tick mark. The [***T***] button opens a Tick Properties window for setting the display options for the Major Ticks and Minor Ticks.

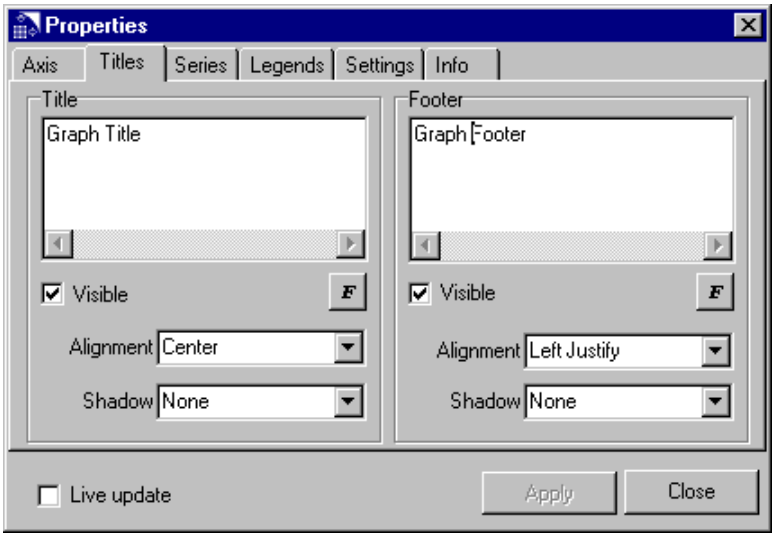


The Logarithm switch changes the axis scale from a normal scale to a logarithmic scale.

The Inverted switch changes the location of the Minimum and Maximum values on the axis. The default axis setting is for the X-axis to increase from bottom to top and the Y-axis to increase from left to right. If the Inverted switch is selected the X-axis increases from top to bottom and the Y-axis increases from right to left.

6.2.2 Titles Settings

The Title settings tab (see figure below) is used to control the content, position and appearance of the Title and Footer for the graph.



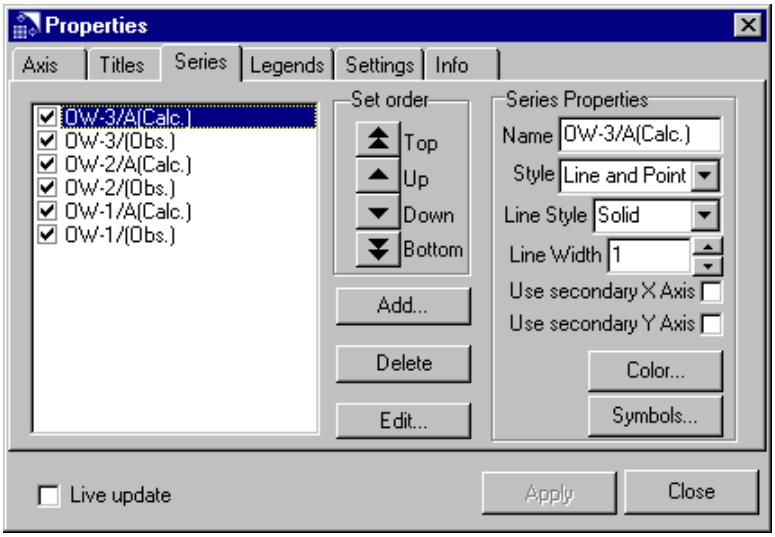
The Visible switch hides/shows the Title or Footer, while the [***F***] button is used to select the desired font, size and color of the text.

The Alignment option controls the position of the Title or Footer text (Left, Center or Right justified).

The Shadow option controls the type of shadow to apply to the text of the Title or Footer (None, Raised or Lowered).

6.2.3 Series Settings

The Series settings tab (see figure below) is used to control the appearance of each data series and how they are plotted on the graph.



The data Series currently available to plot are listed on the left-hand side of the Properties window. A checkmark indicates the active data series which are currently being displayed on the graph.

A data series may be disabled by clicking on the checkbox to remove the checkmark.

The Set order buttons are used to change the appearance order of the series as they are plotted to the screen. The first series in the list is the last series plotted, such that it will 'cover' any prior series plotted to the graph.

The [Add] button is used to add a data series to the graph. This option is described in the section Adding a Data Series on page 271.

The [Delete] button is used to delete the selected data series from the list.

The [Edit] button is used to edit the selected data series. The functionality and features of the Edit Series window is similar to the Add Series window shown on page 271.

The Series Properties frame controls the name and appearance of the selected data series.

The Name field is used in the graph legend to identify the data series on the graph.

The Style option is used to select the style used to plot the data on the graph. The available Style options include:

- Points
- Line
- Line and Point
- Volume
- Arrow
- Piecewise constant

- Area
- Bar

The Line Style and Line Width options are only available if the selected Style includes a line.

The Use secondary X-axis option will plot the X-data for the selected data series using a secondary X-axis located on the right-hand side of the graph.

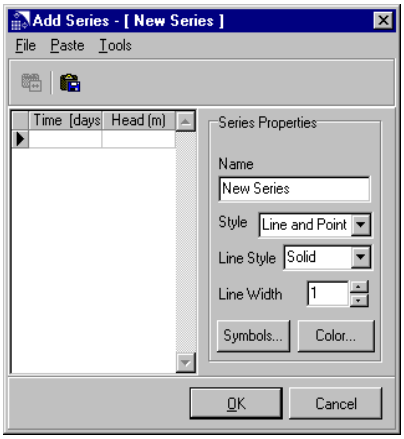
The Use secondary Y-axis option will plot the Y-data for the selected data series using a secondary Y-axis located on the top side of the graph.

The [Color] button is used to select the color of the line used to join the data points of the selected series.

The [Symbols] button opens the Select Symbol window used to select the symbol shape, size, fill color and pen color used to represent the selected data series on the graph.

Adding a Data Series

A data series may be added to the graph by selecting the [Add] button in the Series tab of the graph Properties window. An Add Series window will appear as shown in the following figure.



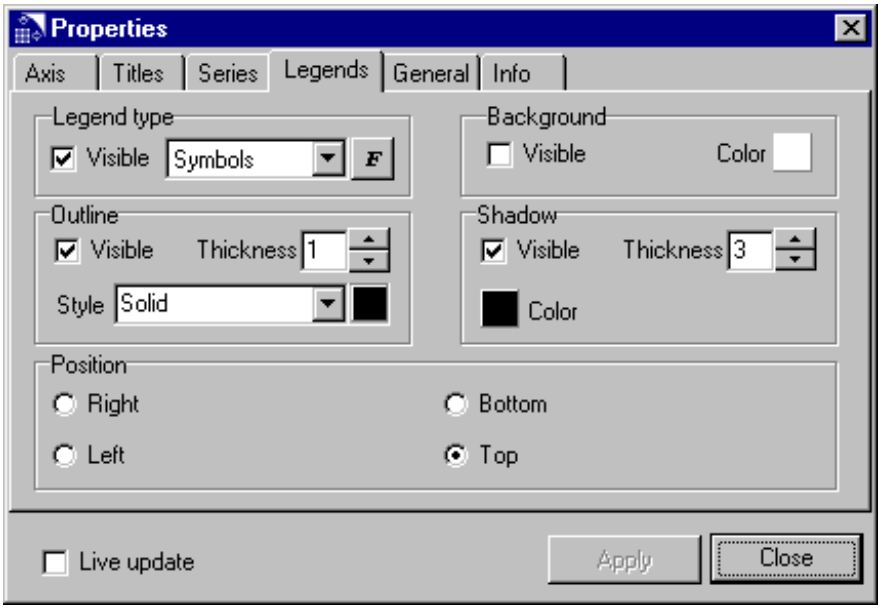
The data for the new series may be added by:

- manually entering data in the table
- importing data from a text file
- pasting data from the clipboard

The Series Properties frame is used to define the name and appearance of the new series as described in the previous section.

6.2.4 Legend Settings

The Legend settings tab (see figure below) is used to control the appearance and position of the legend(s) for the graph.



The Legend type options are used to set the Visible status and text font [***F***] used for the two different types of legends available.

- The Symbols legend displays the data series associated with each symbol on the graph.
- The Color legend displays the color scale associated with the selected data series plotted on a map.

For X-Y scatter graphs, time series graphs, histograms and bar charts the only available Legend type will be Symbols.

The Background options are used to set the appearance properties of the background fill inside the legend box. A

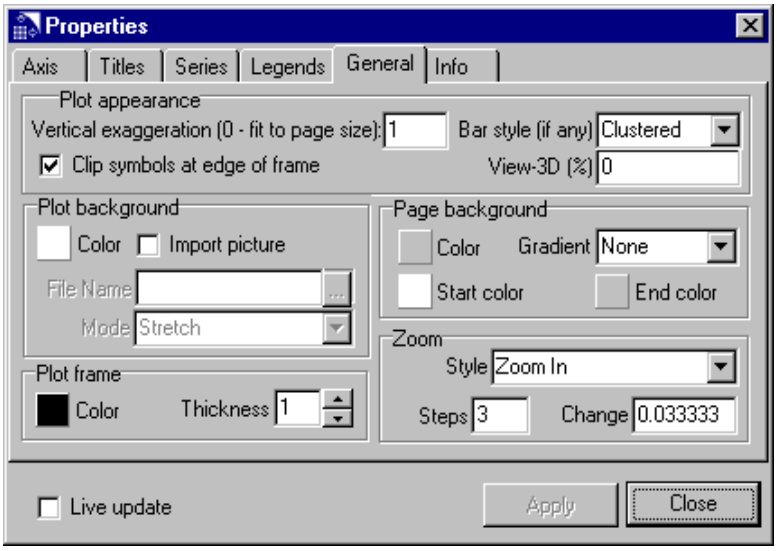
The Outline options are used to set the appearance properties of the outline around the selected legend.

The Shadow options are used to set the appearance properties of the legend box shadow.

The Position options are used to select the legend position outside the graph. The legend may also be positioned anywhere inside the graph by dragging-and-dropping the legend object into the graph area.

6.2.5 General Settings

The General settings tab (see figure below) is used to set the general appearance properties for the graph.



The Plot appearance options are described as follows:

- The Vertical exaggeration is the ratio of the scale of the Y-axis to the scale of the x-axis. If the value is 0, the graph size will be maximized to fit the screen or page. If the value is 1 the X-axis will have the same scale as the Y-axis (but not necessarily the same length).
- The Clip symbols at edge of frame switch will prevent the appearance of the symbol shapes outside of the axes boundary of the graph display area. To prevent this, the minimum/maximum values for the axes are automatically set marginally smaller/larger than the real minimum/maximum for the data.
- The View-3D (%) option displays the graph as a 3D view at an angle. The % value controls the depth of the 3D-View.
- The Bar style option is used to select the style of bar chart to display data series plotted using a bars. The options are Clustered, Z-Ordered, Stacked, and 100% Stacked.

The Plot background options are used to set the appearance properties for the background of the graph within the plot frame.

- The Color box is used to select a solid color to use for the background
- The Import picture switch indicates whether a picture file will be imported to use for a background image.
- The File Name field indicates the name of the picture file.
- The Mode option is used to set the image display mode. Stretch will fit the

image to the entire plot frame area, Fix will maintain the aspect ratio while trying to fit the image to the plot frame area, and Tile will replicate the image throughout the plot frame area.

The Page background options control the appearance of the screen or page behind the graph display area.

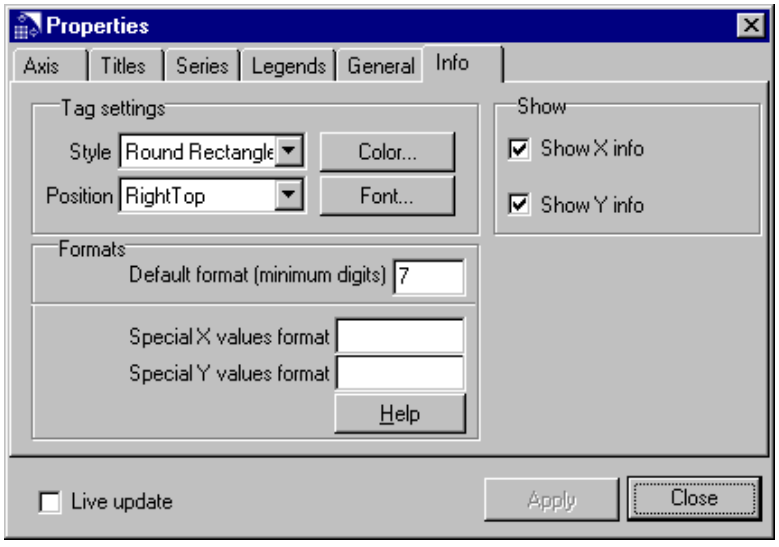
- The Color box is used to select the solid color (only applicable if Gradient = None).
- The Gradient option is used to select the direction of the color gradient (options are either None, Left-Right or Top-Bottom).
- The Start color box is used to select the starting gradient color.
- The End color box is used to select the end gradient color.

The Plot frame options are used to set the appearance properties of the outline around the plot frame.

The Zoom options control the operation of the animated Zoom In and Zoom Out features.

6.2.6 Info Settings

The Info settings tab (see figure below) is used to set the appearance properties for the information tags for selected data points. These tags can be displayed by clicking on a data point in the graph.



The Bubble Settings options are used to set the appearance properties of the information tags on selected data point.

The Style option is used to select from a list of shapes for each tag (options include Round Rectangle No Bubble).

The Position option is used to select the preferred position of the label relative to the data point (options include Right Top, Top Center, Right Bottom, Left Top, Top Center and Left Bottom).

The [Color] button is used to select the fill color for the selected label shape.

The [Font] button is used to select the font, size and color of the label text.

The Show options are used to show/hide the data point values and labels.

Formats

Format specifiers have the following form:

"%" ["-"] [width] ["." prec]

A format specifier begins with a % character. After the % come the following, in this order:

- An optional left justification indicator, ["-"]
- An optional width specifier, [width]
- An optional precision specifier, ["." prec]

The following summarizes the possible values for type:

e = Scientific The value is converted to a string of the form "-d.ddd...E+ddd". The resulting string starts with a minus sign if the number is negative. One digit always precedes the decimal point. The total number of digits in the resulting string (including the one before the decimal point) is given by the precision specifier in the format string--a default precision of 15 is assumed if no precision specifier is present. The "E" exponent character in the resulting string is always followed by a plus or minus sign and at least three digits.

f = Fixed The value is converted to a string of the form "-ddd.ddd...". The resulting string starts with a minus sign if the number is negative. The number of digits after the decimal point is given by the precision specifier in the format string--a default of 2 decimal digits is assumed if no precision specifier is present.

g = General The value is converted to the shortest possible decimal string using fixed or scientific format. The number of significant digits in the resulting string is given by the precision specifier in the format string--a default precision of 15 is assumed if no precision specifier is present.Trailing zeros are removed from the resulting string, and a decimal point appears only if necessary. The resulting string uses fixed point format if the number of digits to the left of the decimal point in the value is less than or equal to the specified precision, and if the

value is greater than or equal to 0.00001. Otherwise the resulting string uses scientific format.

n = Number The value is converted to a string of the form "-d,ddd,ddd.ddd...". The "n" format corresponds to the "f" format, except that the resulting string contains thousand separators.

Conversion characters may be specified in uppercase as well as in lowercase--both produce the same results. For all floating-point formats, the actual characters used as decimal and thousand separators are obtained from the Decimal Separator and Thousand Separator global variables. Index, width, and precision specifiers can be specified directly using decimal digit string (for example "%10d"), or indirectly using an asterisk character (for example "%*.*f"). When using an asterisk, the next argument in the argument list (which must be an integer value) becomes the value that is actually used. For example,

Format('%*.*f', [8, 2, 123.456])

is the same as

Format('%8.2f', [123.456]).

A width specifier sets the minimum field width for a conversion. If the resulting string is shorter than the minimum field width, it is padded with blanks to increase the field width. The default is to right-justify the result by adding blanks in front of the value, but if the format specifier contains a left-justification indicator (a "-" character preceding the width specifier), the result is left-justified by adding blanks after the value.

6.3 Map Properties

IChart may also be used to plot contour maps and color maps of spatially distributed data. IChart maps are currently only available through the VM Engines component for previewing the head, drawdown and concentration results while the simulation is still running.

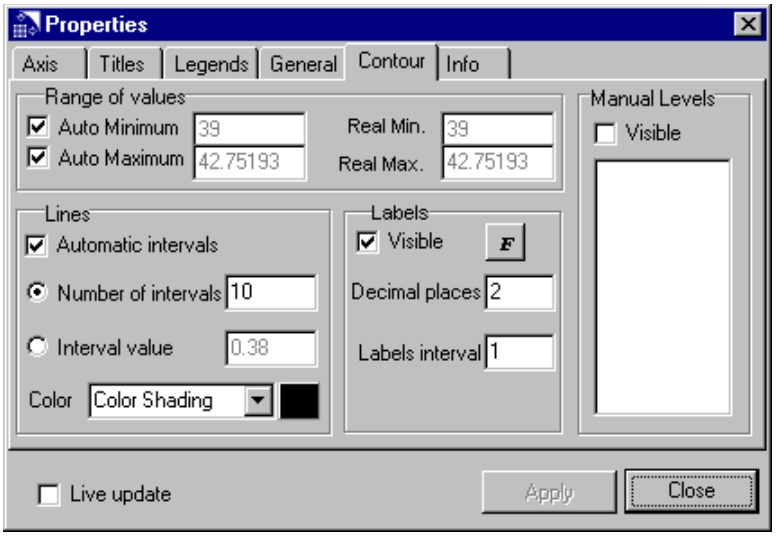
The IChart maps also have some additional icons in the toolbar used specifically for mapping purposes. When a contour map is the active overlay, the following icons will appear on the toolbar.

Color map	Switches from a contour map to a color map
Grid	Shows/hides the finite difference grid.
Animate Pathlines	Animates the particle flow Pathlines.
Annotate	Add text, lines, shapes and arrows to the map.

Overlay Control	Controls the appearance priority of the map overlay.
Y-Cross section	View a cross-section through the grid along the Y-direction.
X-Cross section	View a cross-section through the grid along the X-direction.
Show legend	Shows/hides the symbol legend for the map.
Copy to clipboard	Copies a bitmap image of the map to the Windows clipboard.
Add contour(s)	Add contour line(s) at selected locations by clicking.
Delete contour(s)	Deleted selected contour lines by clicking on them.
2.87 Add/Move labels	Add new labels to contour lines, or drag and drop existing labels to new locations.

6.3.1 Contour Settings

The Contour settings tab (see figure below) is used to set the appearance properties for the contour lines and labels.



The Range of values options are used to set the minimum and maximum contour line values. If the Auto switch is selected the Minimum/Maximum value for the first contour line value will be automatically determined from the Real Min./Real Max. value.

The Lines options are used to select the increment method used to automatically calculate the contour line values to plot on the map.

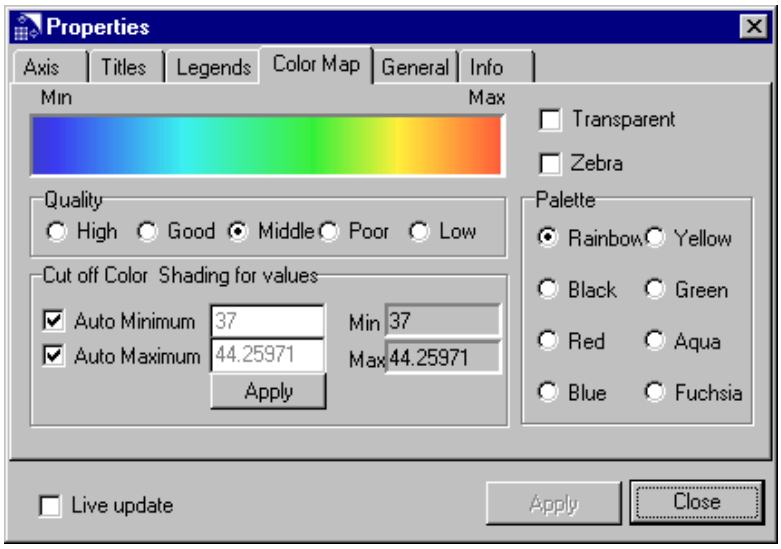
- The Automatic intervals switch will show/hide the automatic contour line values.
- The Number of intervals option will plot a fixed number (N) of contour lines equivalent to the number of intervals. The increment value is calculated taking the different between the Minimum and Maximum contour values and dividing the result by (N-2).
- The Interval value option specifies the contour increment value.
- The Color option is used to set the color of the contour lines. The Solid option will color all contour lines the same color, while the Color Shading option will plot the contour lines using colors which are scales according to the contour value.

The Labels option is used to set the appearance properties of the contour line labels.

- The Visible switch shows/hides labels
- The font [***F***] button is used to select the font, size and color of the labels
- The Decimal places option defines the number of decimal places for each label
- The Labels Interval option labels only every Nth contour line.
- The Manual Levels table is used to enter custom contour line values.

6.3.2 Color Map Settings

The Color Map settings tab (see figure below) is used to set the appearance properties for the color map.



The Transparent switch will set the color map to be semi-transparent such that other features of the map will be visible through the color map.

The Zebra switch will remove the gradation between the different colored zones to display seven distinct colored zones.

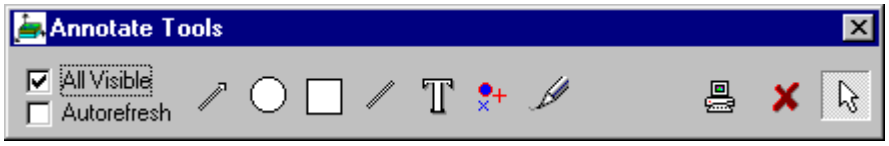
The Quality options are used to select the quality of the color map. The High Quality looks the best, but it takes longer to render and the print.

The Palette options are used to select the colors for the map.

The Range of values option is used to define the minimum and maximum limits of the values plotted. Any values outside of this range will be “clipped” (blanked) from the map display.

6.4 Annotation Tools

The image annotation options can be accessed by selecting **Edit/Annotation**. A floating **Annotation Tools** window will appear on the screen as shown in the following figure.



- Use the button to draw an arrow
- Use the button to draw a circle
- Use the button to draw a rectangle
- Use the button to draw a line
- Use the button to add text
- Use the button to add symbols
- Use the button to sketch a line
- Use the button to refresh the screen
- Use the button to delete a selected annotation object
- Use the button to select, re-size and move the annotation objects

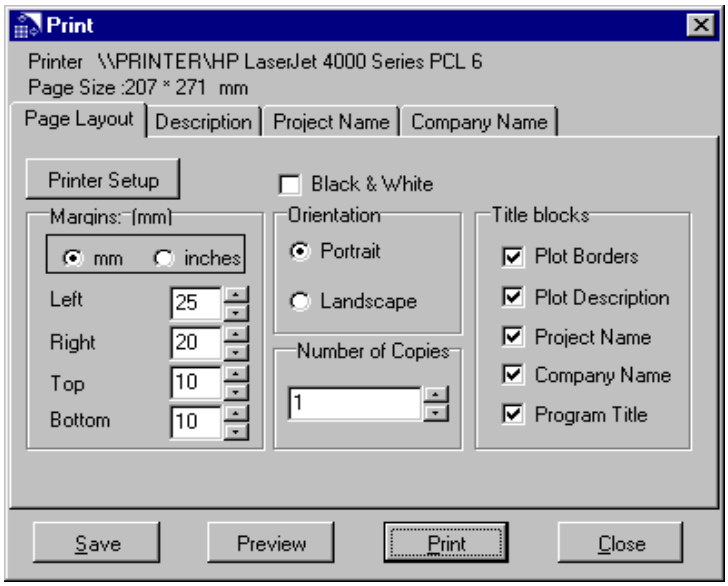
6.5 Printing Options

The IChart graph or map can be printed by selecting File/Print from the top menu bar or by clicking the [Print] icon in the toolbar. The following Print window will appear for setting up the printer and customizing the margins, orientation and appearance of the page. The current printer and page size settings are displayed at the top of the Print window.

The following sections describe the features and functionality of the various printing options.

6.5.1 Page Layout

The Page Layout window is used to setup the printer, set the page margins and orientation, and to "design" the layout of the page title blocks. The various settings for the Page Layout window are described below.



The [Save] button is used to save the Print settings including the Description, Project Name and Company Name.

The [Preview] button is used to show a preview of the page as it will appear when it is printed.

The [Print] button will print the page and close the Print options window.

The [Close] button will close the Print options window.

The **[Printer Setup]** button is used for selecting the destination printer and paper source, paper size and graphics quality options.

The Black and White switch is used to convert all colors in the plot to either black or white. This option may be used to black and white printers if some gray shades are not printing heavy enough or if some details in lighter colors are being missed.

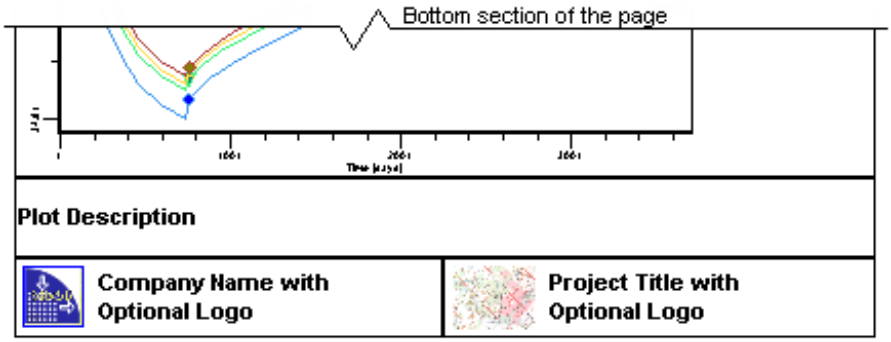
The Margins options are used to set the size of the margins on each side of the selected page size.

The Orientation option is used to select the orientation of the plot on the printed page.

The Number of copies option is used to set the number of copies of the page to print.

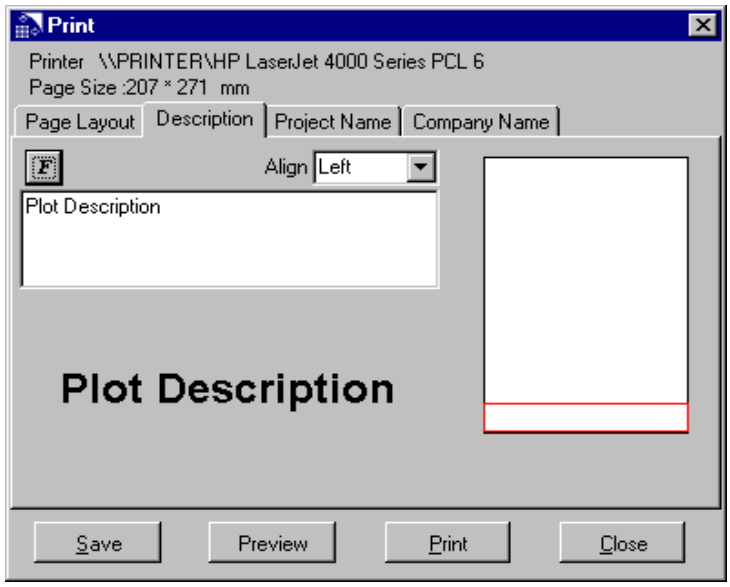
The Title blocks options are used to customize the appearance of the page layout as shown in the following figure (the actual arrangement and size of the title blocks on the page will vary depending on the number of title blocks selected).

- **Plot Borders** will plot an outline along the page margins
- **Plot description** will add a title block to display a description of the plot (see section Plot Description on page 282).
- Project Name will add a title block to display the Project Name and a bitmap logo (see section Project Name on page 283).
- Company Name will add a title block to display the Company Name and logo (see section Company Name on page 284).
- Program Title will add a title block to display the Visual MODFLOW program information.



6.5.2 Plot Description

If the Description option is selected in the Page Layout tab, a Description tab will be active in the Print window as shown in the following figure.



To enter the Description of the plot simply click in the text box and start typing (or editing the current Description). A preview of the Description title block will appear in the space below the Description text box.

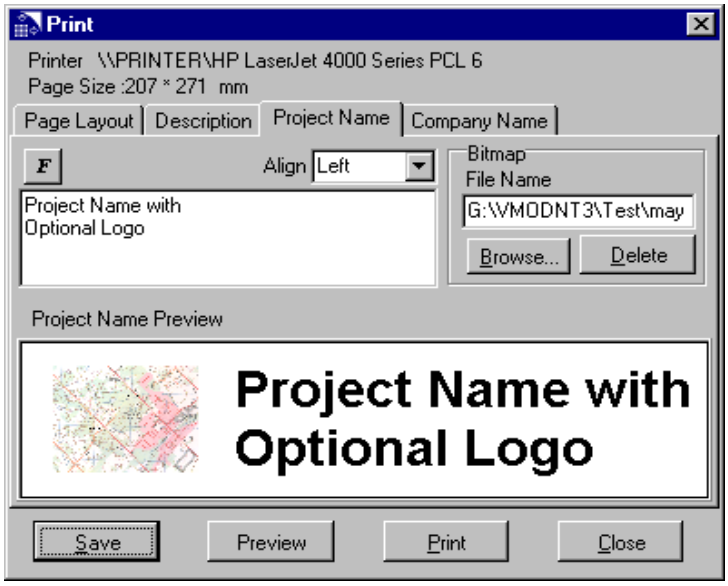
The font [***F***] button is used to select the desired font, size, style and color for the Description text.

The **Align** option is used to align the Description on the **Left**, **Center** or **Right** of the Description title block.

The Description information can be saved for subsequent printing of this information by clicking the [Save] button.

6.5.3 Project Name

If the Project Name option is selected in the Page Layout tab, a Project tab will be active in the Print window as shown in the following figure.



To enter the Project Name simply click in the text field and start typing (or editing the current Project Name).

The font [***F***] button is used to select the desired font, size, style and color for the Project Title text.

The **Align** option is used to align the Description on the **Left**, **Center** or **Right** of the Project Name title block.

The Bitmap option is used to import a bitmap image to display on the left of the Project Name title block. Use the [Browse] button to select the image file or use the [Delete] button to delete the selected image file.

The Project information can be saved for subsequent printing of this information by clicking the [Save] button.

6.5.4 Company Name

If the Company Name option is selected in the Page Layout tab, a Project Title tab will be activated in the Print window as shown in the following figure.

To enter the Company Name simply click in the text field and start typing (or editing the current Company Name).

The font [***F***] button is used to select the desired font, size, style and color for the Company Name text.

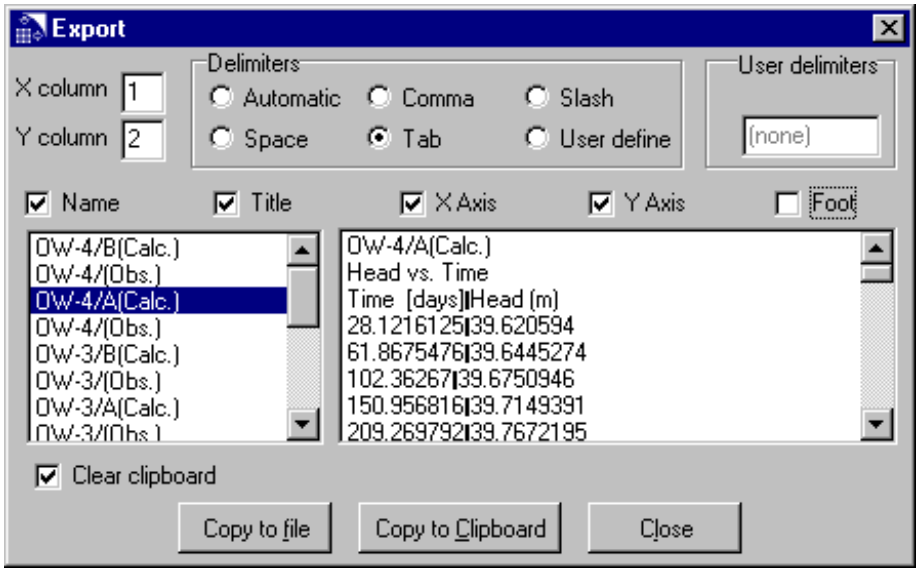
The **Align** option is used to align the Description on the **Left**, **Center** or **Right** of the Company Name title block.

The Bitmap option is used to import a bitmap image to display on the left of the Company Name title block. Use the [Browse] button to select the image file or use the [Delete] button to delete the selected image file.

The Company Name information can be saved for subsequent printing of this information by clicking the [Save] button.

6.6 Exporting Data

The data from each data series in the graph may be exported to an ASCII text file by selecting File/Export ASCII... from the top menu bar or by clicking the [Export Data] icon in the toolbar. The following Export window will appear with options to select the delimiter and titles for the data series being exported.



The Delimiters options are used to select the delimiter to use to separate the X column and Y column data values.

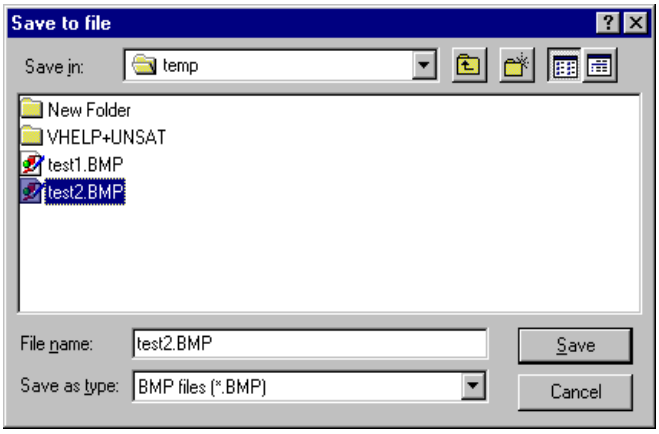
The Name, Title, X-Axis, Y-Axis and Foot checkboxes will show/hide these headers for each data series.

The list of available data series is shown on the left-hand list box, while a preview of the selected data series is shown in the right-hand list box. Multiple data series can be exported in series by holding the <Ctrl> key down while selecting the data series to export.

The [Copy to file] button will write the selected data to an ASCII text file, while the [Copy to Clipboard] button will copy the selected data to the Windows clipboard.

6.6.1 Saving to a Graphics File

The graph or map image displayed can be saved to a graphics file by selecting **File/ Save** as from the top menu bar. The following **Save to file** dialog will appear.



The 3D image can be saved to three different graphics formats:

- **Bitmap file (.BMP)**
- **Windows Metafile (.WMF)**
- **Enhanced Windows Metafile (.EMF)**

Either of these graphics files can be imported into most word processing software packages.

> **Note:** The resolution of the graphics file image will depend on your screen resolution and on the size of the **Image editor** window. In order to maximize the image quality you should maximize the **Image editor** window to full screen.

Alternatively, the image may be copied to the Windows clip board by selecting **Edit/ Copy to Clipboard** from the top menu bar, or clicking the **[Copy to Clipboard]** icon from the top toolbar. This image can be pasted into most word processing and graphics editing programs.

7

Visual MODFLOW 3D-Explorer

The Visual MODFLOW 3D-Explorer is a three-dimensional visualization and animation component for displaying and presenting groundwater flow, pathline and contaminant transport modeling data using a variety of three-dimensional graphical formats. The data structure is similar to that used by Visual MODFLOW and the graphical tools and presentation formats available are specifically designed for groundwater modeling applications.

This chapter provides a detailed description of the features and functionality of the various options for preparing and customizing a three-dimensional presentation of groundwater modeling data. The sections of this chapter are presented as follows:

- Getting Started
- Model Elements and Display Settings
- Creating Slices and Cross-Sections
- Creating Cut-aways
- Creating an Animation
- Saving Scene Configurations
- Printing Options
- Saving to Graphics Files

7.1 Getting Started

The Visual MODFLOW 3D-Explorer (VMOD 3D-Explorer) is designed for the 3D visualization and animation of Visual MODFLOW projects. The VMOD 3D-Explorer can be started directly from within the Visual MODFLOW environment or as a “stand alone” application without Visual MODFLOW running.

To start the Visual MODFLOW 3D-Explorer directly from Visual MODFLOW, click the **[F2-3D]** button located on the lower toolbar of the **Visual MODFLOW** interface. This will open the **VMOD 3D-Explorer** in a separate window, and will load the active Visual MODFLOW project.

To start the VMOD 3D-Explorer as a stand-alone application running outside of Visual MODFLOW, navigate through the Windows Start menu by selecting **Start/Programs/ WHI Software/Visual MODFLOW 2.8.2/ Visual MODFLOW 3D-Explorer.**

This will start the VMOD 3D-Explorer without any project loaded. To load a project, select **File/Open** and navigate to a directory where the desired Visual MODFLOW project (***projectname.vmf***) is located.

Closing the VMOD 3D-Explorer

If the VMOD 3D-Explorer was started directly from Visual MODFLOW, then it should be closed by returning to the **Visual MODFLOW** interface and again clicking the **[F2-3D]** button again.

If the VMOD 3D-Explorer was launched as a stand-alone application without Visual MODFLOW running, then it can be closed by simply clicking the close icon **[X]** in the upper right corner of the window.

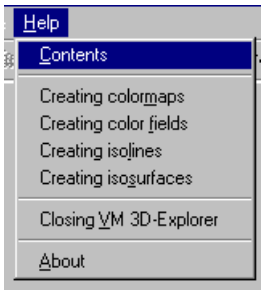
VMOD 3D-Explorer Data Files

The VMOD 3D-Explorer reads the model input data from Visual MODFLOW v.3 data files and it reads the model output data from simulation results files generated by running MODFLOW, MODPATH, and MT3D using the VM Engines. The file formats for the Visual MODFLOW input data files are described in Appendix A, while the file formats generated by MODFLOW, MODPATH, and MT3D are binary files.

The VMOD 3D-Explorer will not properly read input data files or simulation results files generated by earlier versions of Visual MODFLOW or from other modeling software packages.

VMOD 3D-Explorer On-Line Help

VMOD 3D-Explorer on-line help can be accessed in one of two ways. Clicking **Help** on the top toolbar will produce the options shown below:



Selecting **Contents** will produce the table of contents page of the help file. The other selections will jump directly to the help file concerning the selected topic.

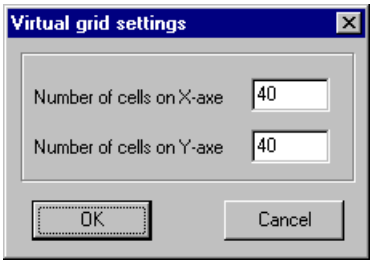
Another way to access the VMOD 3D-Explorer on-line help is to select an interface object and then press the **<F1>** button on your keyboard. This opens the help file for the selected interface object. For example, clicking on a slider in the **Navigate** toolbar then pressing **<F1>** will produce the help file on the **Navigate** toolbar.

Software Performance Considerations

Virtual Grid Settings

If the model has a very large number of grid cells, the VMOD 3D-Explorer may run very slowly during rotations or animations. In this situation the **Virtual Grid** option may be used to increase the speed of the data processing image rendering. The **Virtual Grid** option is used to set up a uniformly spaced grid with a specified number of rows and columns (Note: In order for this option to be useful, the number of rows and columns specified needs to be much smaller than the number of rows and columns in your model). The **Virtual Grid** option will interpolate the data from the model grid to the uniformly spaced virtual grid. This allows a smaller amount of information to be processed much faster. However, this also results in a loss of resolution of the data and some local scale minimum and maximum values may be missed.

To set up a virtual grid for the model, select **Settings/Virtual grid settings** from the top toolbar. A **Virtual grid settings** dialog window will appear as shown in the figure on the right.



Enter the desired number of rows and columns for the virtual grid and then press the **[OK]** button.

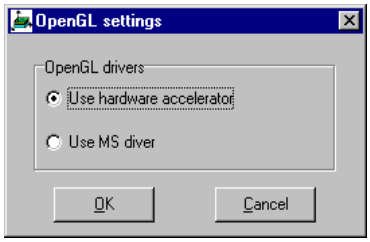
The virtual grid is project specific and the project must be opened again to view the virtual grid.

To open the project with the virtual grid, click **File/Open with virtual grid** from the top toolbar and then select the desired Visual MODFLOW project.

OpenGL Settings

By default, the VMOD 3D-Explorer will attempt to use the vendor provided driver included with graphics acceleration hardware. If problems are encountered with the vendor provided drivers (display/performance inadequate), then VMOD 3D-Explorer provides the option to use the Microsoft Driver for Open GL.

The OpenGL settings can be modified by selecting **Settings/Open GL** from the top menu bar to load the **OpenGL settings** dialog as shown in the following figure.

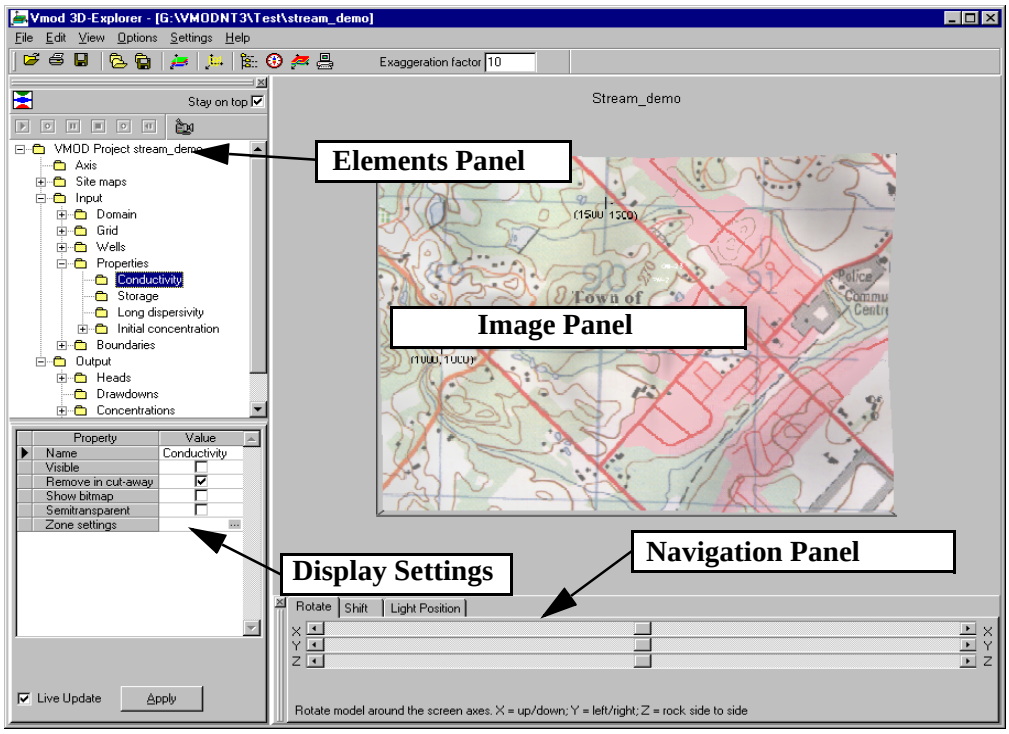


VMOD 3D-Explorer must be closed and re-opened before the new Open GL driver will be used.

7.1.1 About the Interface

The basic layout of the VMOD 3D-Explorer interface is shown in the following figure. The interface consists of four primary components:

- **The Display Screen:** Displays the 3D image of the selected model elements.
- **The Navigation Tools Panel:** Contains a set of navigation tools to control the position and orientation of the 3D image and adjust the light source location.
- **The Model Tree Panel:** A tree structure list of the available model elements and the display settings associated with each element.



Positioning the Panels

The **Model Tree Panel** and the **Navigation Tools Panel** are both “dockable” panels, which means they can be moved and “docked” to another location on the interface, or they can be left as “floating” panels on your Windows desktop (i.e. they not docked to any location on the interface). These panels can either be docked on the left side of the interface or on the bottom of the interface.

Moving a Panel

To move a panel to another location, click on the Drag Bar and drag it to another location (keep the left mouse button pressed down while you drag the panel).

Floating Panels

Once a panel has been moved from the docked position to a floating position, a Title Bar will appear at the top of the panel and it will behaves like a separate Window. The panel window will float on top of the VMOD 3D-Explorer interface as long as it is the active window. The **Model Tree Panel** has an option "**Stay on top**". When this is active, the **Model Tree Panel** will always float on top of the VMOD 3D-Explorer window, even when the VMOD 3D-Explorer is the active window.

Docking Panels

Floating panels can be docked again by clicking the mouse pointer on the panel Title Bar and dragging it to the left or bottom edge of the VMOD 3D-Explorer window. A grey outline will appear when the mouse pointer is in the proper location and the panel is dockable. Release the mouse button to dock the panel at the desired docking area.

Closing Panels

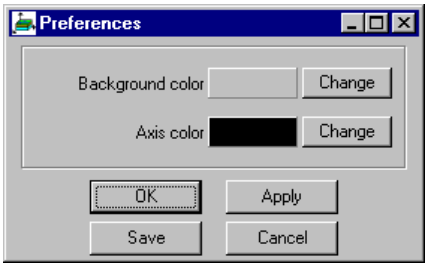
The panels may be removed from the VMOD 3D-Explorer interface by clicking the close icon. The panels can be re-opened using the **View** options from the top menu bar.

View Preferences

The View Preferences currently includes the **Background color** of the **Display Screen**, and the **Axes color**. The default settings for the background color is black, and the default settings for the axes lines is white. The **View Preferences** can be modified by selecting **View/Preferences** from the top menu bar, or by clicking the toolbar icon labelled **View Preferences** icon.

The following **View Preferences** dialog window will appear.

The **Background color** and the **Axis color** can be modified by clicking the **[Change]** button and selecting the desired color. These settings can be saved for future sessions by clicking the **[Save]** button.



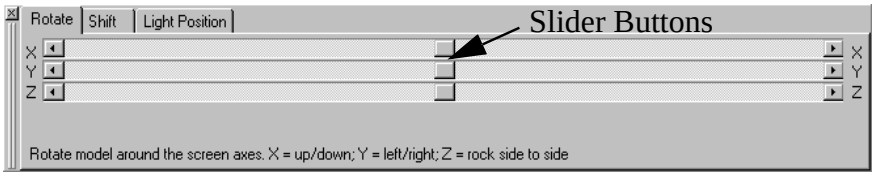
Vertical Exaggeration

The VMOD 3D-Explorer will apply the same vertical exaggeration as specified in the Visual MODFLOW model. This value is displayed in the top toolbar of the **VMOD 3D-Explorer** window as shown in the figure below.

This value can be changed at any time to obtain a more desirable vertical exaggeration of the model.

3D Navigation Tools

The **Navigation Tools Panel** should appear on your screen as shown in the figure below. If the **Navigation Tools Panel** does not appear on the screen, click **View/ Navigate** from the top menu bar and the **Navigation Tools Panel** should appear on the bottom docking area of the **VMOD 3D-Explorer** window:



Alternatively, the **Navigation Tools Panel** can be brought up by clicking the **[Navigate]** icon located on the top toolbar.

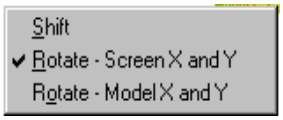
The **Navigation Tools Panel** has three tabs:

- The **Rotate** tab controls the rotation of the 3D image around the X, Y and Z axes of the **Display Screen**.
- The **Shift** tab controls the location of the 3D image along the X, Y and Z axes of the **Display Screen**.
- The **Light Position** tab controls the location of the light source for the 3D image.

The Z-axis is oriented into and out of the **Display Screen**, the X-axis is oriented horizontally left and right across the **Display Screen**, and Y-axis is oriented vertically up and down the **Display Screen**.

The **Slider Buttons** are used to rotate and shift the model around (rotate) or along (shift) the selected axis.

The image orientation and location can also be changed by RIGHT-CLICKING anywhere in the model domain and choosing from one of the following options.



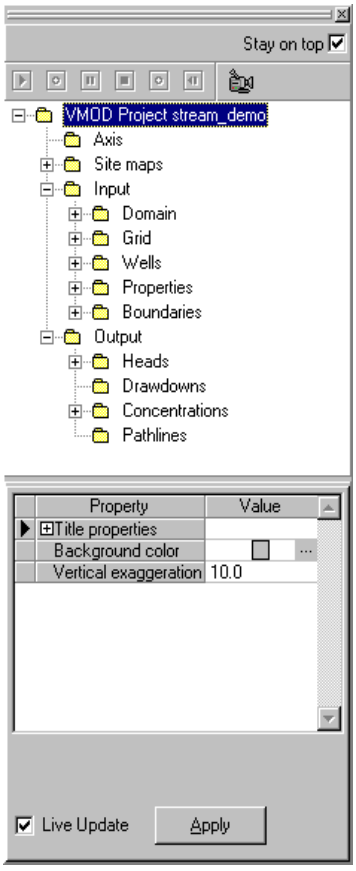
- The **Shift** option allows for translation of the model domain in the plane of the screen by clicking and dragging the mouse pointer in the desired direction.
- The **Rotate - Screen X and Y** rotates the model around the fixed axes of the **Display Screen** by clicking and dragging the mouse pointer along the X or Y direction.
- The **Rotate - Model X and Y** rotates the model around the 3D image axes by clicking and dragging the mouse pointer in the desired rotation direction.

The view can be returned to the default view settings at anytime by clicking the **Reset scene position** icon located on the top toolbar.

7.2 Model Elements and Display Settings

The **Model Tree Panel** should appear as shown in the following figure. If the **Model Tree Panel** is not visible, click **View/Model Tree** from the top menu bar or click the **Model Tree** icon.

The upper section of the **Model Tree Panel** contains a tree structured list of the model elements which can be visualized, while the lower section of this panel contains a table of the **Display Settings** for the selected model element. The **Model Tree Panel** can be used to selectively view model elements, or alter the display settings of selected model elements.



The **Model Tree** is structured in a hierarchical fashion where model elements within the tree can be expanded by clicking on the "**+**" symbol. The structure is very similar to the menu structure used in Visual MODFLOW, so it should seem pretty familiar.

Each model element listed in the **Model Tree** has an associated list of "Display Settings" that can be accessed by selecting (clicking) the model element from the **Model Tree**. A brief description of each display property is available by clicking the mouse pointer on the display property. This produces a tool tip (description of the property) in the bottom of the **Model Tree Panel** (below the **Display Settings** table).

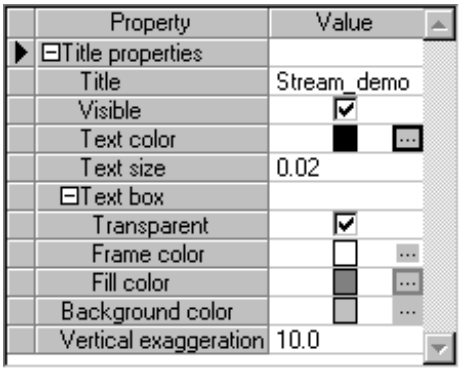
Although each model element has a different set of display settings, there are several display settings which are common to most model elements.

- **Visible** - Shows/hides the selected model element [On/Off]
- **Name** - Sets the name of the model element as it appears in the **Model Tree**
- **Color** - Sets the RGB display color of the model element
- **Remove in cutaway** - Hides/shows the model element in a 3D cutaway zone
- **Semitransparent** - Transparency setting of the selected model element
- **Show bitmap** - Drapes the site map image onto the selected model element

The following is a brief description of the various model elements and the display settings for each model element listed in the **Model Tree**.

VMOD Project Display Settings

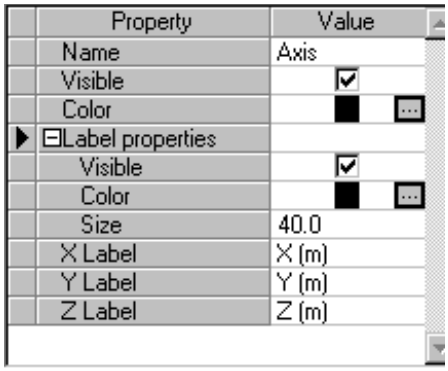
The **VMOD Project** element consists of general project settings as shown in the following figure.



By default, the project **Title** is given the same name as the model and appears at the top of the **Display Screen**. The can be moved to any location within the **Display Screen** by clicking on the **Title** and dragging it to a new location.

Axis Properties

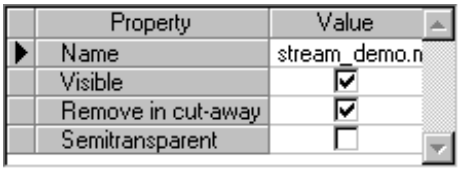
The **Axis** model element controls the appearance of the lines and labels for the X, Y and Z axes. The axes are primarily used to indicate the total dimensions (size) of the 3D image and to orient the image when it has been rotated.



The default axes labels indicate the axes direction and the units, but this can be customized to display alphanumeric text.

Sitemaps Display Settings

The VMOD 3D-Explorer supports both AutoCAD .DXF files and bitmap image files. The **Sitemaps** category contains a list of the sitemaps used in the Visual MODFLOW model. and control the display settings for each individual sitemap.



In cases where the sitemap is not appearing clearly because of the colors used in the DXF file, you can specify a fixed color to apply to all lines and attributes of the DXF file.

7.2.1 Input Model Elements

The **Input Class of** model elements is structured similar to the **Input** section of Visual MODFLOW whereby the model elements are grouped into different categories consisting of the primary building blocks of a groundwater model:

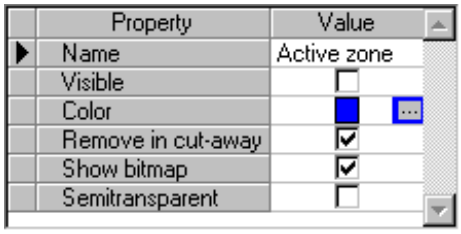
- **Domain**
- **Grid**
- **Wells**
- **Properties**
- **Boundaries**

Each of these model element categories contains a selection of model elements with consistent display settings as described below.

Domain Display Settings

The Domain category contains the following model elements:

- **Active Zone**
- **Inactive Flow**
- **Inactive Transport**



Each of these model elements has the same set of display settings as shown in the figure on the right.

The **Active Zone** model element displays a colored ‘blanket’ around the model grid cells that are ‘active’ in the model. The active grid cells are the cells which are used in the calculations for the flow model.

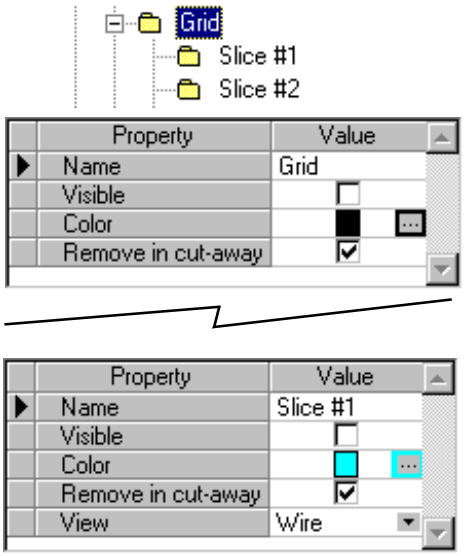
The **Inactive Flow** model element displays a ‘blanket’ around the model grid cells designated as inactive in the Visual MODFLOW model. These **Inactive Flow** grid cells are not used in the calculation of the flow model.

The **Inactive Transport** model element displays a ‘blanket’ around the model grid cells designated as inactive for mass transport in the Visual MODFLOW model. These **Inactive Transport** grid cells are not used in the calculation of the mass transport model.

Grid Display Settings

The **Grid** model element displays gridlines for the entire three-dimensional finite difference grid. However, since this is usually impractical for visualization/ interpretation purposes, the **Grid** model element also contains a list of N horizontal **Grid Slice** elements, where NL is equal to the number of model layers.

The **Grid Slice** elements display the grid lines on a 2D horizontal slice through the selected layer of the model.

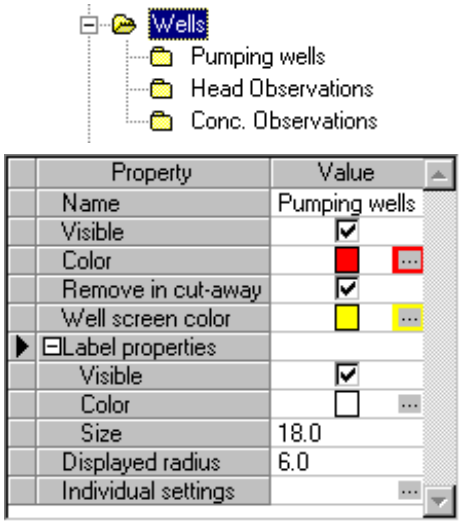


Wells Display Settings

The model elements in the **Wells** category corresponds to the different types of wells available in a Visual MODFLOW project including:

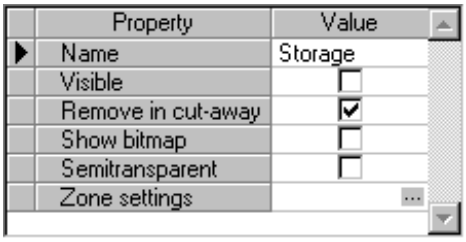
- **Pumping wells**
- **Head Observations**
- **Conc. Observations**

The display settings for each type of well can be controlled as a group using the display settings shown in the figure on the right, or individually by clicking the **[...]** button in the **Individual settings** field.



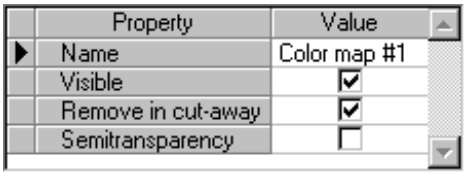
Properties Display Settings

The model elements in the **Properties** category corresponds to the different types of properties in a Visual MODFLOW project as shown in the figure on the right. For properties related to different types of contaminant species (e.g. Initial concentrations) a sub-list of model elements corresponding to each species will be provided.



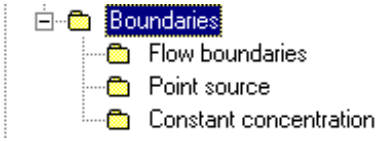
In Visual MODFLOW, each of these Properties elements are defined in terms of zones, where each zone has a specified set of values associated with it. As in Visual MODFLOW, each zone is displayed as a solid color in each cell. The display settings of these model elements can be controlled as a group using the display settings shown on in the figure on the right, or the individual zone settings for each Properties element can be controlled by clicking the **[...]** button in the **Zone Settings** field.

Properties Color Maps

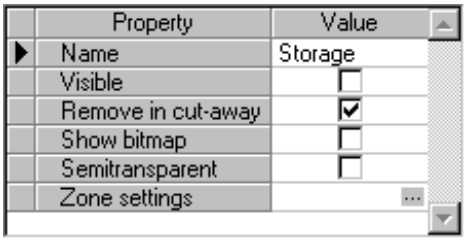


The Properties data can also be plotted using a Color map on any vertical or horizontal slice through the model by clicking the **Add Color map** icon above the **Model Tree** and choosing the desired slice location. The Properties **Color map** will use the same zone color settings as defined in the **Zone settings** for each Properties element.

Boundaries Display Settings

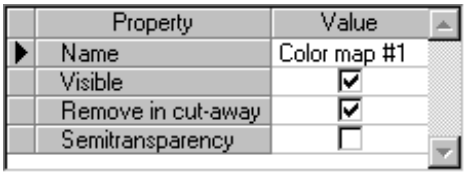


The model elements in the **Boundaries** category corresponds to the different types of boundary conditions in a Visual MODFLOW project as shown in the figure on the right. The **Flow Boundaries** element controls the display settings for all flow-related boundary conditions. By default, each of the flow-related boundary condition types are displayed using the same color settings as in Visual MODFLOW. However, the display settings for each boundary condition type can be controlled by clicking the **[...]** button in the **Zone Settings** field.



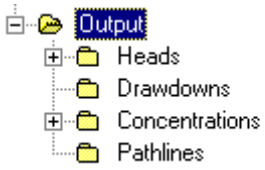
Boundaries Color Maps

The Boundaries data can also be plotted using a Color map on any vertical or horizontal slice through the model by clicking the **Add Color map** icon above the **Model Tree** and choosing the desired slice location. The Boundaries **Color map** will use the same zone color settings as defined in the **Zone settings** for each Boundaries element.



7.2.2 Output Model Elements

The **Output** class of model elements contains four different data categories generated by a Visual MODFLOW model:



- **Heads**
- **Drawdowns**
- **Concentrations**
- **Pathlines**

Each of these **Output** elements has a specific set of display settings as discussed in the following sections.

Heads Display Settings

The **Heads** results for the model can be displayed using the following display elements:

- **isosurface** (see **Isosurfaces** on page 304)
- **color map** (see **Color Maps** on page 307)
- **contour map** (see **Contour Maps** on page 309)
- **color field** (see **Color Fields** on page 311)

Please refer to the respective sections for instructions on how to create these display elements and for details on the display settings associated with each one.

The **Heads** display settings controls the global settings for all display elements under the **Heads** category.

The **Palette** option controls the color scale used on all **Heads** display elements. A description of the **Palette** options is provided in the **Color Palette** section on page 312.

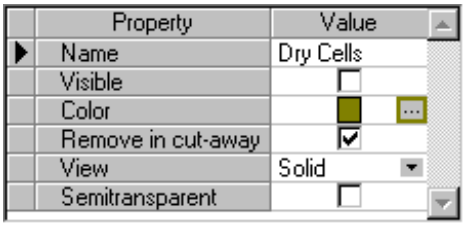
The **Auto reset palette** option will reset the color scale every time a new element is added and for every output time step. For transient data it is best to leave this option off so the color scale won't change with time.

The **Color legend** settings are used to modify the appearance of the color legend as it applies to all **Head** display elements. A description of the **Color legend** options is provided on page 313.

The **Time** setting contains a list of the available output times for the **Heads** results. This option is applicable only for transient simulations and is used to select the desired Output time data to plot on each **Heads** display element.

Dry Cells Display Settings

The **Dry Cells** element is listed under the **Heads** category because the dry cells are determined by the head values in each cell. Therefore, the **Time** setting for the **Heads** also updates the **Dry Cells**.

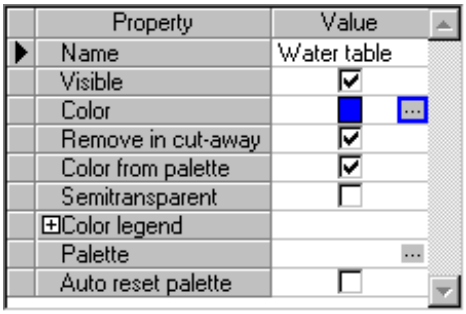


The **Dry Cells** are displayed as solid colored blocks in grid cells where the modeled head value is below the bottom elevation of the grid cell.

Water Table Display Settings

The **Water Table** element is listed under the **Heads** category because the water table elevation is naturally controlled by the simulated head values. Therefore, the **Time** setting for the **Heads** also updates the **Water table**.

The **Water Table** element plots a 3D planar surface at the location of the water table (occurring in cells where the head is equal to the elevation). By default, the **Water table** surface will be set to a uniform color as defined in the **Color** setting. However, the **Color from palette** option will create a Water table color map with the colors scaled according to the water table elevation.

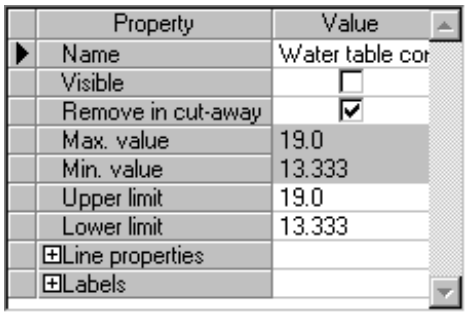


If the **Color from palette** option is selected, a separate **Color legend** will appear for the **Water table Color map** and the **Palette** option can be used to customize the color scale.

Water Table Contour Map

The **Water Table** can also be displayed using a **Contour map** of water table elevations plotted on the **Water table** surface element.

The **Water table contour map** settings can be used to customize the appearance of the contour lines and labels. A detailed description of the **Contour map** display setting is provided on page 309.



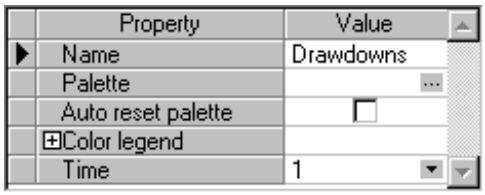
Drawdowns Display Settings

The **Drawdowns** results for the model can be displayed using the following display elements:

- **isosurface** (see **Isosurfaces** on page 304)
- **color map** (see **Color Maps** on page 307)
- **contour map** (see **Contour Maps** on page 309)
- **color field** (see **Color Fields** on page 311)

Refer to the respective sections for instructions on how to create these display elements and for details on the display settings associated with each one.

The **Drawdowns** display settings controls the global settings for all **Drawdowns** display elements.



The **Palette** option controls the color scale used on all **Drawdowns** display elements. A description of the **Palette** options is provided in the **Color Palette** section on page 312.

The **Auto reset palette** option will reset the color scale every time a new element is added and for every output time step. For transient data it is best to leave this option off so the color scale won't change with time.

The **Color legend** settings are used to modify the appearance of the color legend as it applies to all **Drawdowns** display elements. A description of the **Color legend** options is provided on page 313.

The **Time** setting contains a list of the available output times for the **Drawdowns** results. This option is applicable only for transient simulations and is used to select the desired **Output** time data to plot on each **Drawdowns** display element.

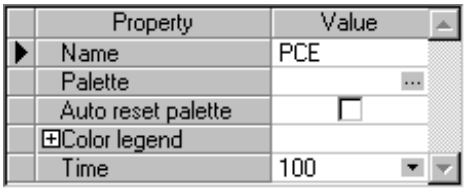
Concentrations Display Settings

The **Concentrations** data category contains of a list of each concentration species from the model. The **Concentrations** results for each species can be displayed using the following display elements:

- **isosurface** (see **Isosurfaces** on page 304)
- **color map** (see **Color Maps** on page 307)
- **contour map** (see **Contour Maps** on page 309)
- **color field** (see **Color Fields** on page 311)

Refer to the respective sections for instructions on how to create these display elements and for details on the display settings associated with each one.

The **Concentrations** display settings for each species controls the global settings for all **Concentrations** display elements.



The **Palette** option controls the color scale used on all **Concentrations** display elements. A description of the **Palette** options is provided in the **Color Palette** section on page 312.

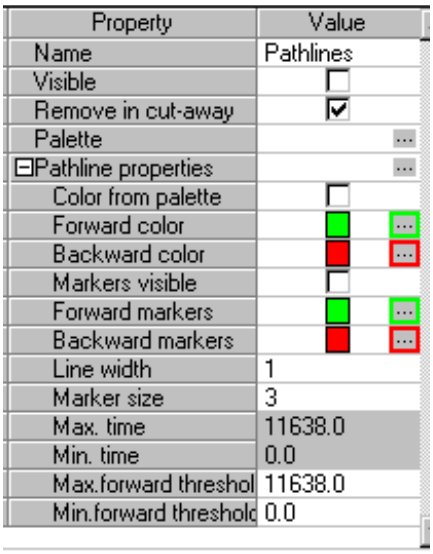
The **Auto reset palette** option will reset the color scale every time a new element is added and for every output time step. For transient data it is best to leave this option off so the color scale won't change with time.

The **Color legend** settings are used to modify the appearance of the color legend as it applies to all **Concentrations** display elements. A description of the **Color legend** options is provided on page 313.

The **Time** setting contains a list of the available output times for the **Concentrations** results. This option is applicable only for transient simulations and is used to select the desired Output time data to plot on each **Concentration** display element.

Pathlines

The 3D flow **Pathlines** elements are displayed using thin lines which can be modified in terms of the line color and thickness as shown in the figure on the right and described below.



- **Color from palette** colors each pathline using scaled colors to indicate the travel time along the pathline
- **Forward color** sets the color of all forward tracking pathlines (unless Color from palette is used)
- **Backward color** sets the color of all backward tracking pathlines (unless Color from palette is used)
- **Markers visible** hides/shows the time markers on all pathlines
- **Forward markers** sets the color of each marker on the forward tracking pathlines
- **Backward markers** sets the color of each marker on the backward tracking pathlines
- **Line width** sets the line width of all pathlines
- **Marker size** sets the size of all markers on all pathlines
- **Max. time** is the maximum travel time for all pathlines
- **Min. time** is the minimum starting time for all pathlines (usually this is 0.0)
- **Max. forward threshold** is the maximum travel time displayed for all pathlines
- **Min. forward threshold** is the minimum travel time displayed for all pathlines

Pathline Output Times

Sections of pathline can be displayed for specified time intervals using the **Max. forward threshold** and **Min. forward threshold** fields.

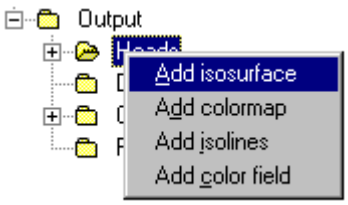
7.2.3 Isosurfaces

An isosurface is a 3D planar surface defined by a constant parameter value in 3D space. Isosurfaces are typically used for demonstrating the spatial distribution of a selected parameter. For groundwater modeling purposes, isosurfaces are generally used for representing the spacial distribution of heads, drawdowns and concentrations.

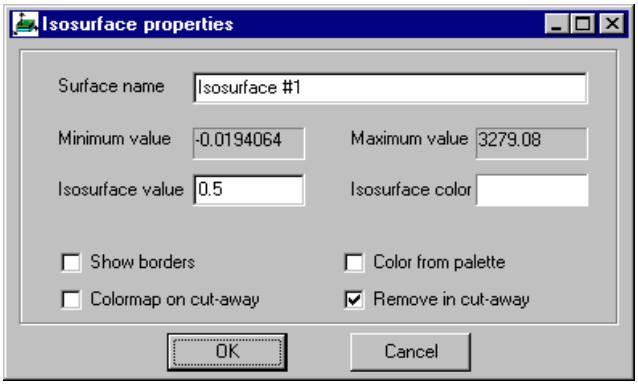
The VMOD 3D-Explorer allows you to create and simultaneously display multiple isosurfaces for the Heads, Drawdowns and Concentrations model elements. In each case, the display settings of the isosurface will be the same regardless of which model element is being displayed.

Creating Isosurfaces

To create an isosurface, click-on the desired element in the **Model Tree** to highlight it, then RIGHT-CLICK on the element and select **Add Isosurface** from the dropdown list. Alternatively, isosurfaces may be created by highlighting the desired element and clicking the **[Add isosurface]** icon located above the **Model Tree**.



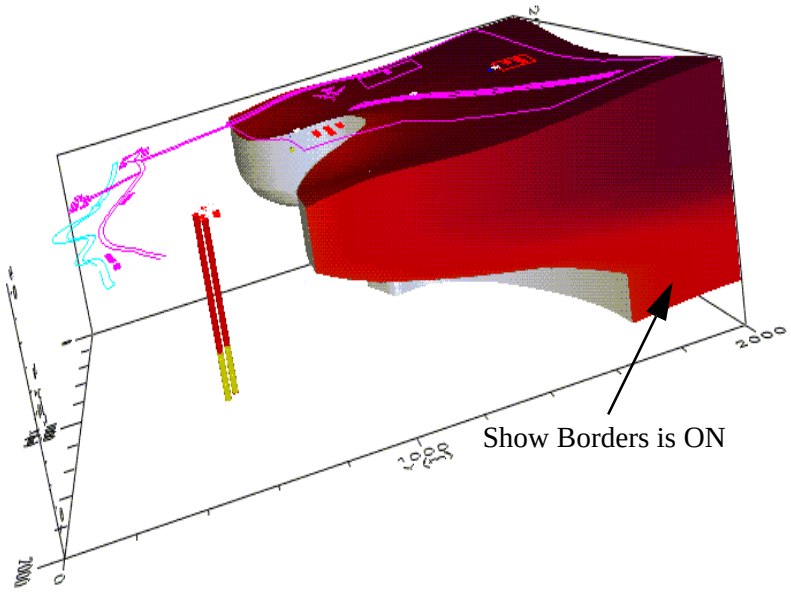
This will open the **Isosurface Properties** window as shown in the following figure.

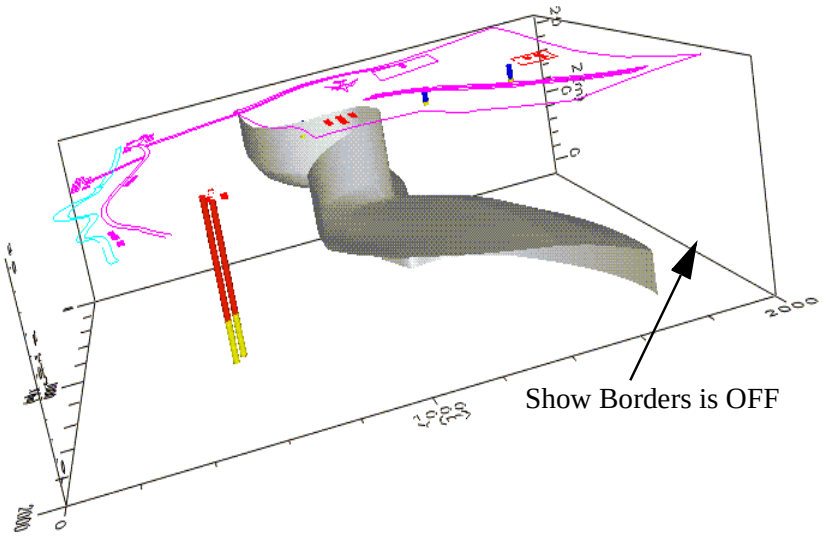


This window is used to set the display settings of the isosurface as described below.

- **Surface name** defines the name of the isosurface as it will appear in the Model Tree under the selected element
- **Minimum value** is the global minimum value of the element for all grid cells and all time steps
- **Maximum value** is the global maximum value of the element for all grid cells and all time steps
- **Isosurface value** is the element value for which the isosurface will be created

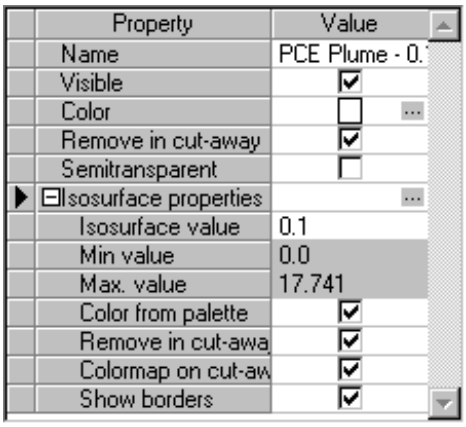
- **Isosurface color** is the user-specified color of the isosurface (double-click color box to customize the color)
- **Show borders** will display a color map of the element values on the borders (sides) of the model domain when the isosurface intersects the edge of the model domain (see the figure below)
- **Color map on cut away** will display a color map of the element values on the section of the isosurface that is removed by the cutaway region
- **Color from palette** will use the element color palette to automatically color the isosurface according to the specified isosurface value
- **Remove in cutaway** will remove the isosurface in a cutaway region


Show Borders is ON


Show Borders is OFF

Isosurface Display Properties

Once the isosurface is created the display settings will appear as shown in the figure on the right.



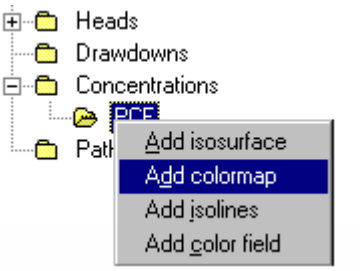
- **Isosurface value** is the value of the selected data type for which the isosurface will be created
- **Min. value** describes the global minimum value of the data type for all grid cells and all time steps
- **Max. value** describes the global maximum value of the data type for all grid cells and all time steps
- **Color from palette** indicates the isosurface color will be automatically determined from the color palette for the selected data type.
- **Colormap on cut away** will display a color map of the data values on the section of the isosurface that is removed by a cutaway slice
- **Show borders** will display a color map of the data values on the borders (sides) of the model domain when the isosurface intersects the edge of the model domain

7.2.4 Color Maps

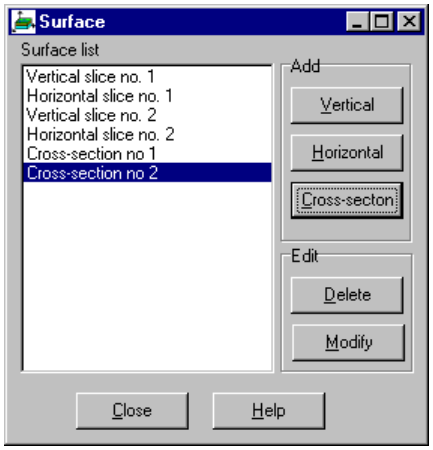
The Color maps elements for the Output **data** (Heads, Drawdowns and Concentrations) will plot distributed colors according to the value of the selected data type in each grid cell along the selected slice. A color legend for the Color map will also appear in the top left-hand corner of the **Display Screen**.

Creating a Color Map

To create a colormap, click-on the desired element in the **Model Tree** to highlight it, then RIGHT-CLICK on the element and select the **Add colormap** option from the dropdown list. Alternatively, isosurfaces may be created by highlighting the desired element and clicking the **[Add colormap]** icon located above the **Model Tree**.



This will open the **Surface** window with a list of the available surfaces (slices). The colormap for the selected model element can be plotted on any of the surfaces listed.



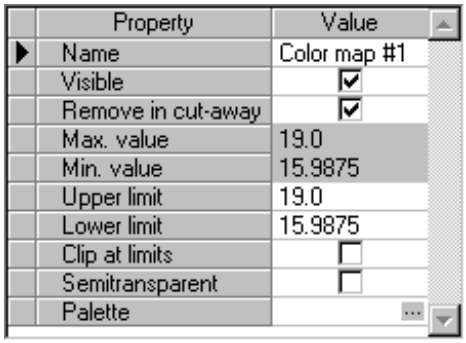
If there are no slices in the list, then this dialog can be used to create the desired vertical, horizontal and cross-section slices to use for plotting Color maps and Contour maps. Please refer to the **Creating Slices** section on page 314.

To select a surface from the list, click-on the desired surface and then click the **[Close]** button.

A color map of the model element distribution will then appear on the selected surface a **Colormap** element will be added to the **Model Tree** under the selected model element.

Color Map Display Settings

Once the Color map element has been added to the Model Tree, the display settings can be customized as described below.



- **Max. value** is the maximum value for the selected data type in the grid cells corresponding to the selected slice.
- **Min. value** is the maximum value for the selected data type in the grid cells corresponding to the selected slice.
- **Upper limit** is the data value above which the color map may be clipped out.
- **Lower limit** is the data value below which the color map may be clipped out.
- **Clip at limits** indicates whether the color map will clipped out above the **Upper limit** and below the **Lower limit**.
- **Palette** is used to customize the data values associated with each color. Any changes made to the color palette for the selected data type will be applied to all color-scaled elements for the selected data type. This ensures that each element uses a consistent color scheme (and a correct color legend) for each data type throughout the entire model. The color palette options are discussed in more detail in **The Color Palette** section on page 312.

7.2.5 Contour Maps

Contour maps are a set of lines plotted on a surface whereby each line is connect by a set of points having equal values of a given data type.

Creating Contour Maps

To create a **Contour map** click-on the desired element in the **Model Tree** and then RIGHT-CLICK on the element and select the **Add contour map** option from the dropdown list. Alternatively, isosurfaces may be created by highlighting the desired element and clicking the **[Add contour map]** icon located above the **Model Tree**.

This will open the **Surface** window with a list of the available surfaces (slices). The colormap for the selected model element can be plotted on any of the surfaces listed.

If there are no slices in the list, then this dialog can be used to create the desired vertical, horizontal and cross-section slices to use for plotting Color maps and Contour maps. Please refer to the **Creating Slices** section on page 314.

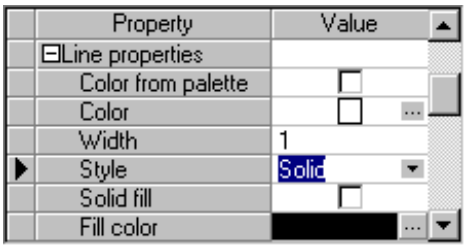
To select a surface from the list, click-on the desired surface and then click the **[Close]** button.

A color map of the model element distribution will then appear on the selected surface a **Contour map** element will be added to the **Model Tree** under the selected model element.

Contour Map Display Settings

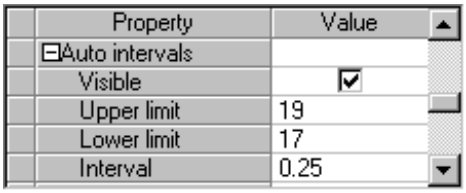
Once the **Contour map** element has been added to the **Model Tree**, the display settings can be customized as described below.

Line properties



- **Color from palette** indicates each contour line will be colored according to the contour line value using the color palette for the selected data type.
- **Color** indicates the solid color used for all contour lines (used only if **Color from palette** is not selected). The browse button can be used to change the current **Color** setting to any RGB color.
- Width is the contour line width
- Style indicates the line style used to plot each contour line (choose from Solid, Dashed, and Dotted).
- **Solid fill** indicates whether the space between the contour lines will be filled with a solid color
- **Fill color** indicates the color of the solid fill between contour lines.

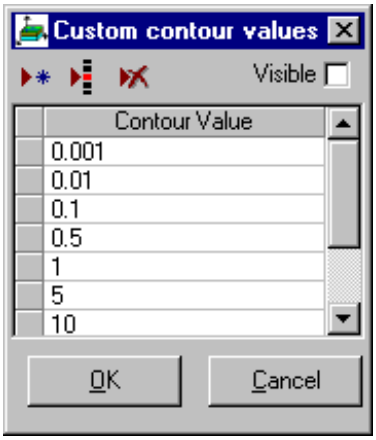
Auto Intervals



- **Upper Limit** is the maximum data value above which no contour lines will be plotted
- **Lower limit** is the minimum contour line below which no contour line will be plotted
- **Interval** is the increment value at which contour lines will be plotted, starting from the Lower limit value

Custom values

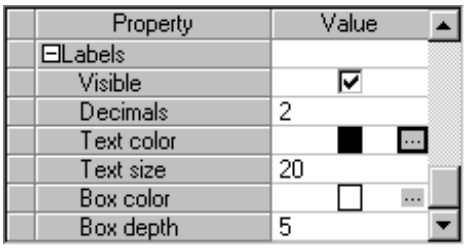
The **Custom Values** setting is used to assign custom contour values in addition to, or in replacement of the regular interval contour values. Press the browse button [...] to load the **Custom contour values** dialog as shown on the right.



- Click to add a value
- Click to insert a value
- Click to delete a value

This setting is commonly used to set logarithmic contour interval values for concentration data.

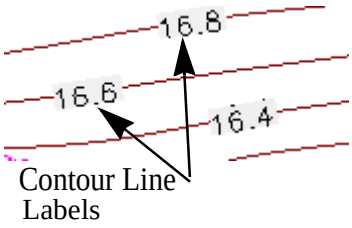
Labels



The **Labels** setting is used customize the appearance of the contour labels.

- **Decimals** is the number of decimals used for each label value
- **Text color** is the color of each label
- **Text size** is the size of each label

The labels are plotted on the top and bottom surface of a flat 3D rectangular box. The size of the box will be automatically adjusted to fit the text size, but the **Box color** and **Box depth** can be customized.

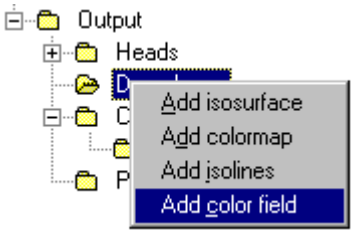


In situations where the 3D planar surface is highly variable in shape, some of the isoline labels may be difficult to read. This is a limitation of the current version of the VMOD 3D-Explorer, but it is a feature that will be improved in later versions.

7.2.6 Color Fields

The **Color fields** display format creates a 3D field of colored points on a user-specified grid. Each point is colored according to the value of the selected model element at each point location. Currently, color fields can be created for **Heads**, **Drawdowns**, and **Concentrations** data.

To create color field, click-on the desired element in the **Model Tree** to highlight it, then RIGHT-CLICK on the element and select the **Add color fields** option from the dropdown list. Alternatively, color fields may be created by highlighting the desired element and clicking the **[Add color fields]** icon located above the **Model Tree**.

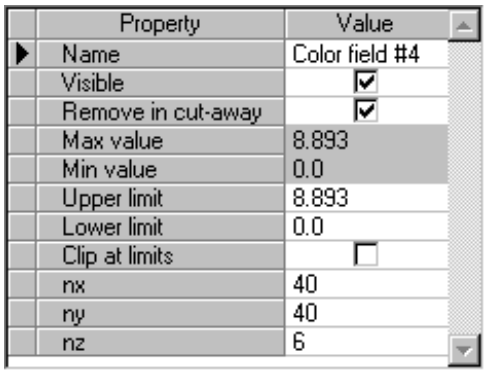


7.2.7 Color Field Display Settings

Once the **Contour map** element has been added to the **Model Tree**, the display settings can be customized as described below.

- **Upper limit** is the data value above which the color field points may be clipped out (not displayed)
- **Lower limit** is the data value below which the color field points may be clipped out (not displayed)

- **Clip at limits** indicates whether the color fields will clipped out (not displayed) above the **Upper limit** and below the **Lower limit**.
- **nx** is the number of color field points in the x-direction
- **ny** is the number of color field points in the y-direction
- **nz** is the number of color field points in the z-direction



7.2.8 The Color Palette

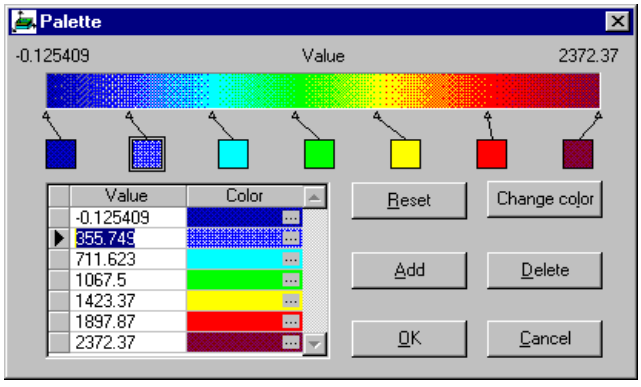
The color **Palette** is used to customize the range of colors used to represent the values of selected model element for each display object. Currently, the color **Palette** is used only for the Model **Output** Elements:

- **Heads** (color scaled head values and water table elevations)
- **Drawdowns** (color scaled drawdown values)
- **Concentrations** (separate color scales for each species)
- **Pathlines** (color scaled travel times)

The color **Palette** settings for each of these model **Output** elements will govern the color scaling used on each display object, including isosurfaces, colormaps, isolines, and color fields.

The color **Palette** settings can be modified by selecting one of the model **Output** elements and clicking the **[...]** button in the **Palette** field of the **Display Settings** table. The following **Palette** dialog window will appear.

The default color setting contains a rainbow of seven colors ranging from a dark blue at the minimum value to a dark red at the maximum value. This range of colors and the values associated with each will be reflected in the **Color Legend** for the selected model **Output** element.



Changing Color Values

The parameter values associated with each color can be easily changed by typing in a new value, or by clicking on one of the color boxes beneath the color bar, and dragging the arrow to a new location on the color bar.

Changing Colors

The color for each color box can be easily modified by selecting the color box and then clicking the **[Change color]** button, or by clicking the **[...]** button for the color you would like to change. Each color can be selected from an RGB 16 million color palette.

Adding Color Intervals

To have more than seven color increments, additional colors can be added to the color scale by clicking on one of the colors in the color value table and then clicking the **[Add]** button. A new color entry will be added with a value midway between the previous and next value.

Deleting a color

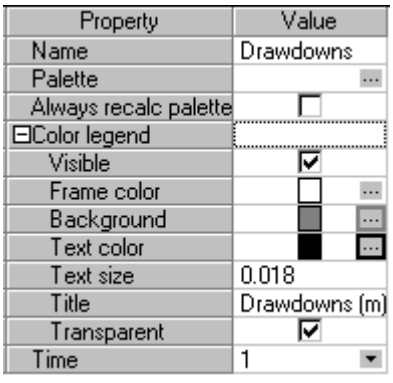
To have fewer color increments, simply remove a color by selecting the color from the **Color Value** table and then clicking the **[Delete]** button.

Resetting the Color Palette

The color settings can be reset to the initial default values by clicking the **[Reset]** button.

7.2.9 The Color Legend

The **Color Legend** is a scale of the element values associated with each color. The values and colors shown in the **Color Legend** are defined by the **Color Palett**e settings for the selected data type Element (see previous section).



Other display settings, including **Title**, **Text size**, **Text color** and **Frame color**, can be easily customized using the display settings options indicated in the figure on the right.

The color legend will automatically appear in the top left-hand corner of the **Display Screen** whenever a display object using the color palette is plotted (e.g. colormap). It can be moved to any other location in the **Display Screen** by dragging-and-dropping it at the desired location.

7.3 Creating Slices and Cross-Sections

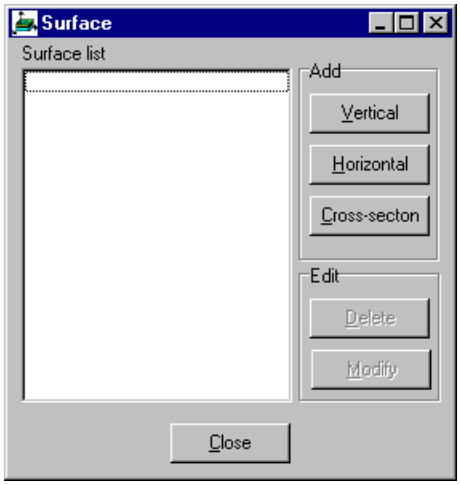
A slice is defined as a 3D planar surface extending horizontally or vertically through the model domain. There are three types of slice objects available:

- **Vertical slices** along the XZ or YZ plane of the model extending through the entire depth of the model.
- **Horizontal slices** along the XY plane of the model
- **Cross-section slices** along a straight line or an irregular polyline through the entire depth of the model

These slice objects define the locations where Colormaps and contour maps can be plotted for selected model elements including **Properties**, **Heads**, **Drawdowns a**nd **Concentrations**. Slices can also be used to define Cutaway regions.

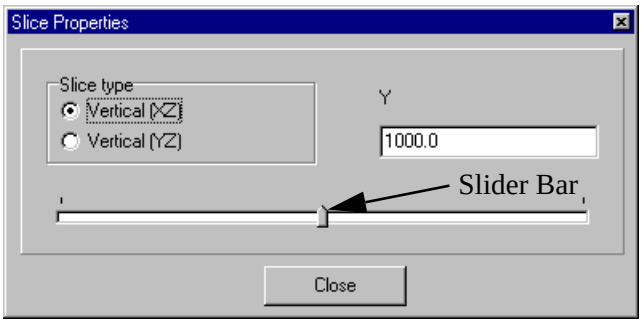
To define the slice locations, select **Options/Define Slices** from the top menu bar, or the **[Define slices]** icon. A **Surface** dialog window will appear as shown below.

The **Surface** dialog window displays a list of the available slices which have been previously defined. The **Surfaces** dialog also has options to create additional slices, or to modify/delete existing slices.



7.3.1 Creating a Vertical Slice

To create a vertical slice through the model domain, lick the **[Vertical]** button to open the **Slice Properties** window as shown in the following figure. A yellow outline of the vertical slice will appear in the **Display Screen**.



The **Slice type** options defines the planar orientation of the slice:

- **Vertical XZ** refers to the plane along the X-axis extending through the entire depth of the model
- **Vertical YZ** refers to the plane along the Y-axis extending through the entire depth of the model

For a **Vertical XZ** slice, then the **Slider Bar** moves the vertical slice along the Y-axis, and the Y-axis value is displayed in the field labelled "**Y**". Alternatively, a Y-axis value can be typed directly into this field.

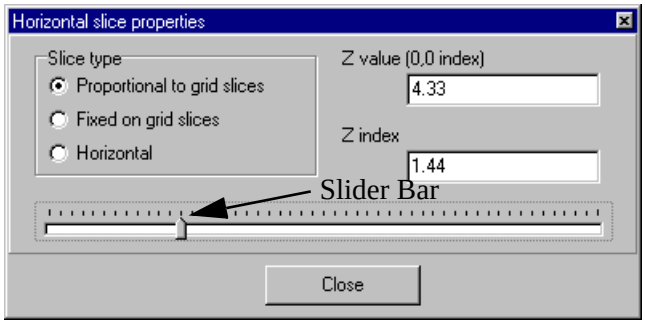
For a **Vertical YZ** slice, then the **Slider Bar** moves the vertical slice along the X-axis, and the X-axis value is displayed in the field labelled "**X**". Alternatively, an X-axis value can be typed directly into this field.

When the desired location for the vertical slice has been defined, click the **[Close]** button to save the vertical slice type and location.

The new vertical slice will appear in the **Surfaces** window.

7.3.2 Creating a Horizontal Slice

To create a horizontal slice through the model domain, click the **[Horizontal]** button to open a **Horizontal slice properties** window as shown below. A yellow outline of the horizontal slice will appear in the **Display Screen**.



The **Slice type** options define the planar orientation of the slice:

- **Proportional to grid slices** allows you to select a horizontal plane through the model that deforms according to the layer surface elevations
- **Fixed on grid slices** allows you to select a horizontal plane corresponding to the selected layer surface
- **Horizontal** allows you to select a flat horizontal plane at a specified elevation

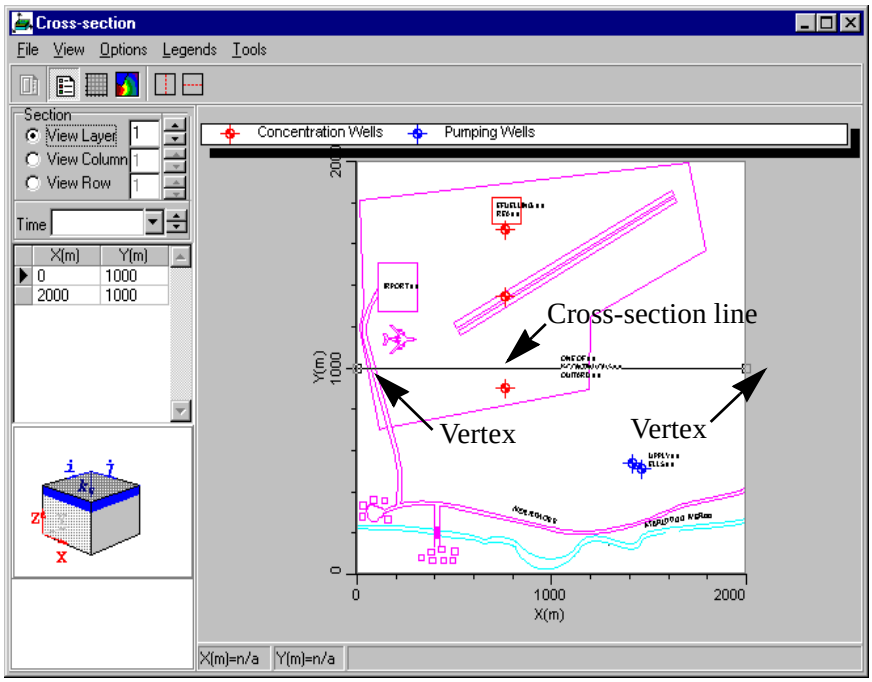
The **Slider Bar** moves the horizontal slice along the vertical Z-axis, and the corresponding slice elevation and layer number are displayed in the fields labelled **"Z value"** and **"Z index**", respectively.

When the desired location for the horizontal has been selected, click the **[Close]** button to save the slice type and location.

The new horizontal slice will appear in the **Surfaces** window.

7.3.3 Creating a Vertical Cross-Section

To create a vertical cross-sections through the model domain click the **[Cross-section]** button to open the **Cross-section** window as shown below. This window displays a map view of the model domain with the associated sitemaps and a default cross-section line extending from the left side of the model to the right side of the model.



The cross-section line defines the location of the cross-section slice.

Moving the Cross-Section Line

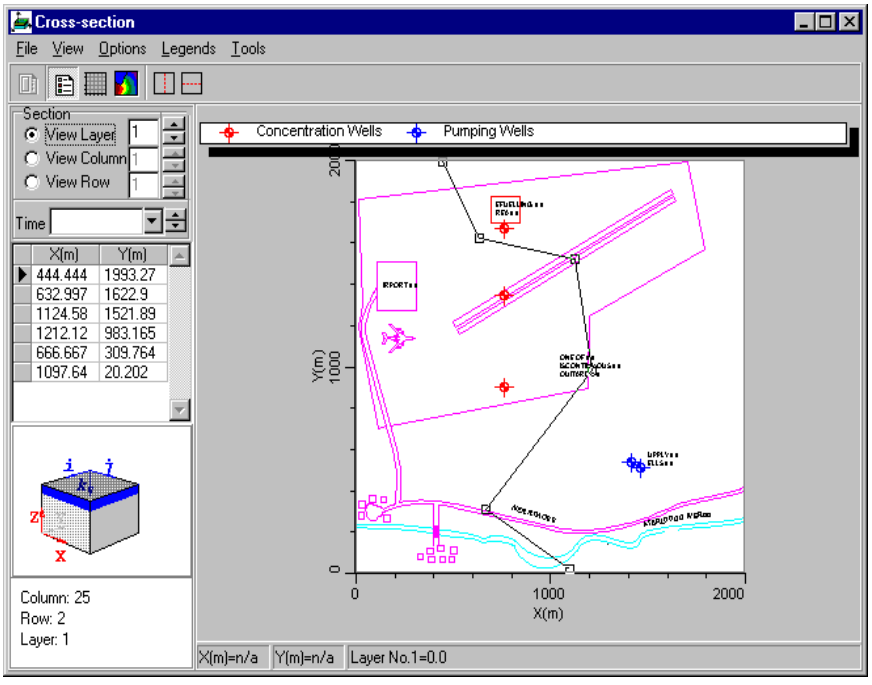
The cross-section line can be moved to a different location by clicking and dragging the horizontal line to a different horizontal location in the model domain.

Changing the Direction of the Cross-Section Line

The cross-section line is not limited to X and Y model axes directions. The cross-section line can be defined along any direction in the horizontal plane by clicking and dragging a cross-section line vertex to a new location within the model domain.

Changing the Shape of the Cross-Section Line

The cross-section line is not limited to a straight line through the model. A cross-section polyline can be defined with many different vertices. By right clicking the cross-section line, a **vertex** can be added to the line, and this new vertex can be dragged anywhere in the model domain. The cross-section created can be jagged and extend anywhere in the model domain as shown in the figure below:



Once the cross-section line has been defined, click **File/Close** to add the vertical cross-section slice to the **Surface list**.

7.3.4 Deleting a Slice

If many different slices have been defined during the current session and the list is becoming too long and cumbersome to work with, any entry in the **Surface list** can be deleted by highlighting the slice in the list and clicking the **[Delete]** button.

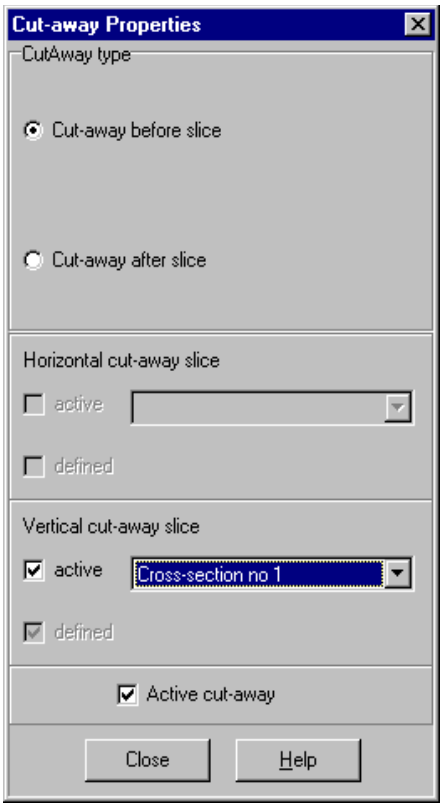
7.3.5 Moving a Slice

The location or orientation of any slice can be modified by highlighting the target slice in the list and clicking the **[Modify]** button. This will cause the **Slice Properties** window to appear where the desired changes can be made.

7.4 Creating Cut-aways

A Cut-away is a section of the 3D image that is removed or blanked out, thus allowing a view of the "inside" of the model domain. The section of the model that is "cut-away" can be defined by any vertical slice or cross-section, or by any flat horizontal slice, or by a combination of the a horizontal and vertical slice.

To create a Cut-away view for the model, select **Options/Select cut-away** from the top menu bar, or click the **Select cut-away** icon in the toolbar. A **Cut-away Properties** window will appear as shown in the following figure.



The **Cut-away Properties** window is used to select the slice defining the section of the model being cut-away, and to choose which side of the model will be removed.

For a **Vertical cut-away slice**, the **Cut-away type** options are:

- **Cut-away before slice** - will remove the section of the image towards the front of the screen
- **Cut-away after slice** - will remove the section of the image towards the back of the screen

For a **Horizontal cut-away slice**, the **Cut-away type** options are:

- **Cut-away above slice** - will remove the section of the image towards the top of the screen
- **Cut-away below slice** - will remove

the section of the image towards the bottom of the screen

For a combined **Vertical cut-away slice** and **Horizontal cut-away slice**, the **Cut-away type** options are:

- **Cut-away before and above slices** - will remove the section of the image towards the front and top of the screen
- **Cut-away before and below slices** - will remove the section of the image towards the front and bottom of the screen
- **Cut-away after and above slices** - will remove the section of the image towards the back and top of the screen
- **Cut-away after and below slices** - will remove the section of the image towards the back and bottom of the screen

The checkbox beside the **Vertical cut-away** slice field and the **Horizontal cut-away slice** field will automatically be set to ON when a slice has been selected. If the active checkbox is set to OFF, the cut-away will not be applied to the image.

7.4.1 Creating an Animation

The VMOD 3D-Explorer allows time-varying modeling results to be animated in order to show the changes in heads, drawdown, and concentration with time. The animation tool shows a sequential progression of the model data from the available output times for each data set. This animation can be saved to an .AVI file for convenient demonstrations using a compatible .AVI file player.

The Animation tools can be activated by highlighting the desired data type (**Heads**, **Drawdowns** or **Concentrations**) in the **Model Tree.** The following toolbar will appear above the **Model Tree**.

Note: The current version of VMOD 3D-Explorer only allows a single data type to be animated at any given time. As such, the **Heads** and **Concentrations** cannot be animated together. Future versions of VMOD 3D-Explorer will have an option to synchronize the data for simultaneous animation.

The **Play** button starts animating the results for the selected data type starting from the current time step.

The **Pause** button pauses the animation at the current time step.

The **Stop** button stops the animation at the current time step.

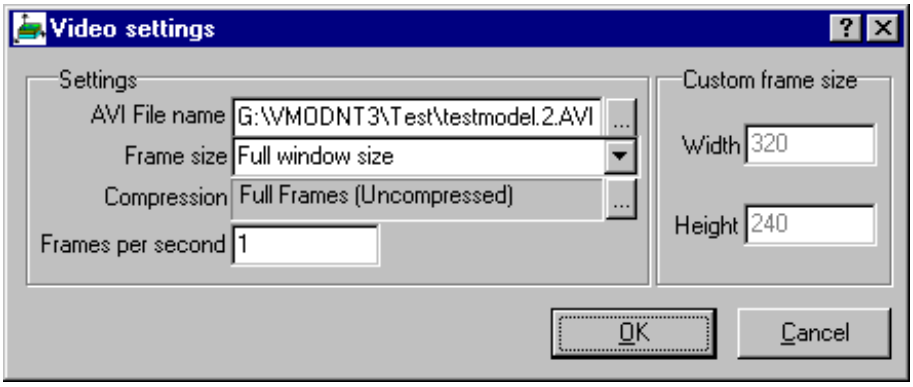
The **Loop** button will repetitively loop through all of the time steps.

The **Rewind** button will set the time to the first time step.

Recording AVI Files

The animation of the simulation results in VMOD 3D-Explorer can be saved to an .AVI file for easy replay using any .AVI compatible media software.

To create an .AVI file click the **Record** button in the **Animation** toolbar. A **Video settings** window will appear as shown in the following figure.



The default **AVI File name** is *modelname*.#.AVI

where,

- *modelname* is the name of the Visual MODFLOW model
- # is an integer number that increments for each AVI file created for the current model

The **AVI File name** can be modified to any path and filename needed by clicking the [...] button.

The **Frame size** setting has a selection of four options:

- **Full window size**
- **640x480**
- **320x240**
- **Custom**

If the **Custom** option is chosen, the **Custom frame size** fields (**Width** and **Height**) will be activated and a frame size can be defined.

The **Compression** setting provides a selection of the various video compression techniques. A higher compression quality will reduce the AVI file size but it will also reduce the quality of the image.

The **Frames per second** setting defines the number of frames (time steps) will be displayed each second in the AVI file.

Playing AVI Files

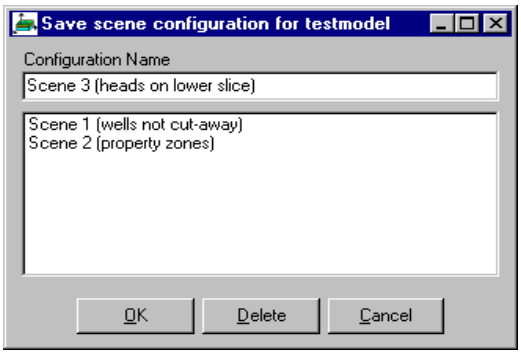
The VMOD 3D-Explorer can preview one of the saved AVI files by clicking the **Show Video** button in the Animation toolbar.

7.5 Scene Configurations

When using the VMOD 3D-Explorer to display and animate model data it is important to be able to save the various display settings for fast and easy recall during a presentation or for comparing different modeling scenarios with the same data set. The VMOD 3D-Explorer is able to save the model display settings by selecting **File/Save Scene configuration** from the top menu bar or by clicking the **[Save Scene Configuration]** icon.

This will bring up the **Save Scene Configuration** dialog window as shown below.

Type the desired name of the scene in the **Configuration Name** field and then press the **[OK]** button.



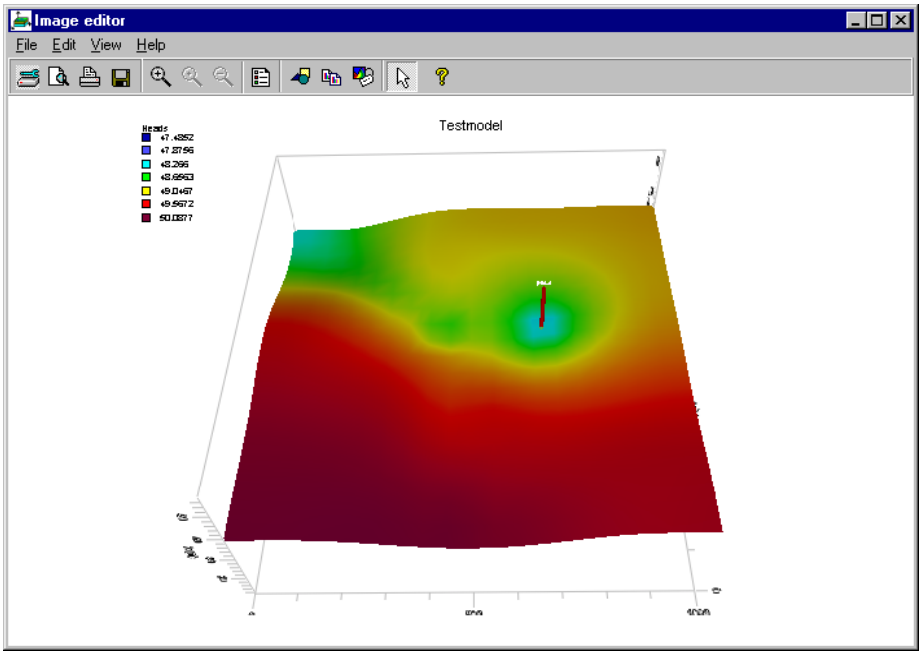
This scene configuration (including attributes, model rotations and shifts) can be loaded during a later session by selecting **File/Load scene configuration** from the top menu bar, or by clicking the **[Load scene configuration]** icon.

Note: Scene configurations saved with a virtual grid may only be restored if the project was opened with the **Open with virtual grid command**.

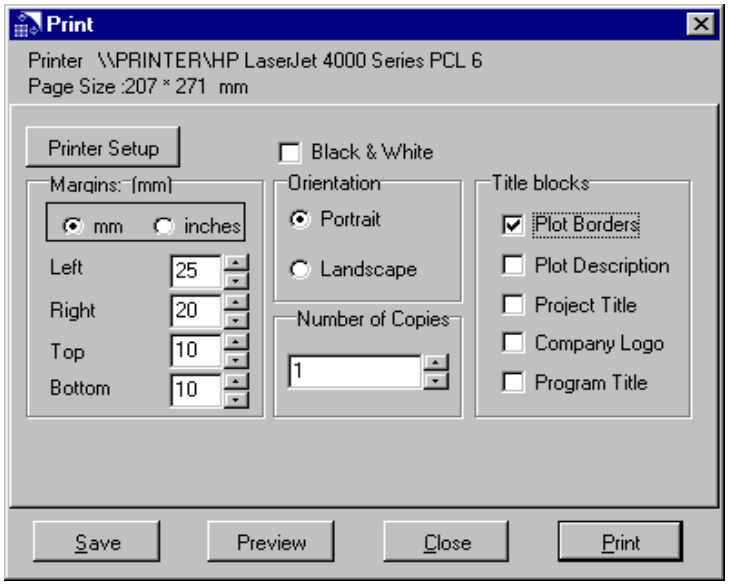
7.6 Printing the 3D Image

Once the desired view of the model has been created, the printing options can be accessed by selecting **File/Print,** or by clicking the **[Print]** icon on the top toolbar.

An **Image editor** window will appear with a preview of the 3D image as is will appear on the printed page (see figure below). This window is used to fine-tune the appearance of the image by adding some text or drawing on the image using the annotation tools described in the section Annotation Tools on page 328.

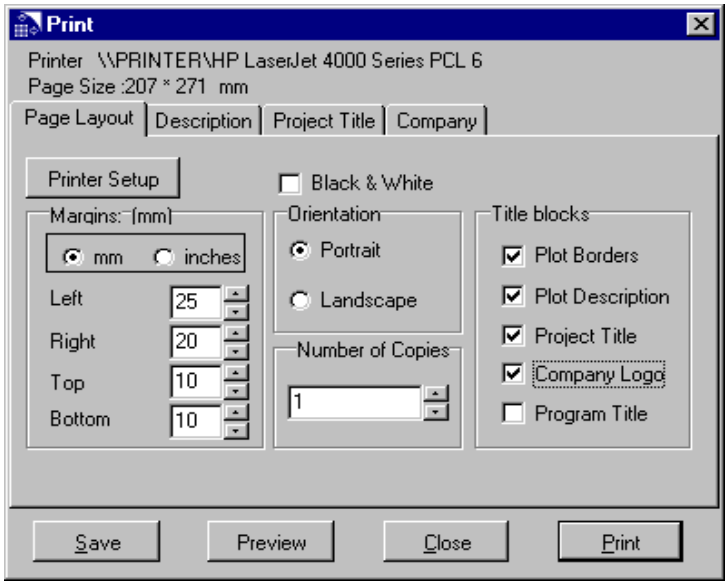


To print the image, select **File/Print** from the top menu bar or click the **[Print]** icon in the toolbar. The following Print window will appear for setting up the printer and customizing the margins, orientation and appearance of the page. The current printer and page size settings are displayed at the top of the Print window. The following sections describe the features and functionality of the various printing options.



7.6.1 Page Layout

The Page Layout window is used to setup the printer, set the page margins and orientation, and to “design” the layout of the page title blocks. The various settings for the Page Layout window are described below.



The [Save] button is used to save the Print settings including the Description, Project Name and Company Name.

The [Preview] button is used to show a preview of the page as it will appear when it is printed.

The [Print] button will print the page and close the Print options window.

The [Close] button will close the **Print** options window.

The **[Printer Setup]** button is used for selecting the destination printer and paper source, paper size and graphics quality options.

The Black and White switch is used to convert all colors in the plot to either black or white. This option may be used to black and white printers if some gray shades are not printing heavy enough or if some details in lighter colors are being missed.

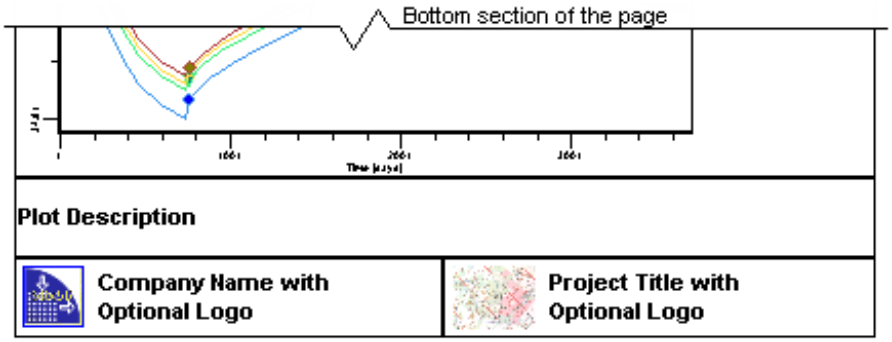
The Margins options are used to set the size of the margins on each side of the selected page size.

The Orientation option is used to select the orientation of the plot on the printed page.

The Number of copies option is used to set the number of copies of the page to print.

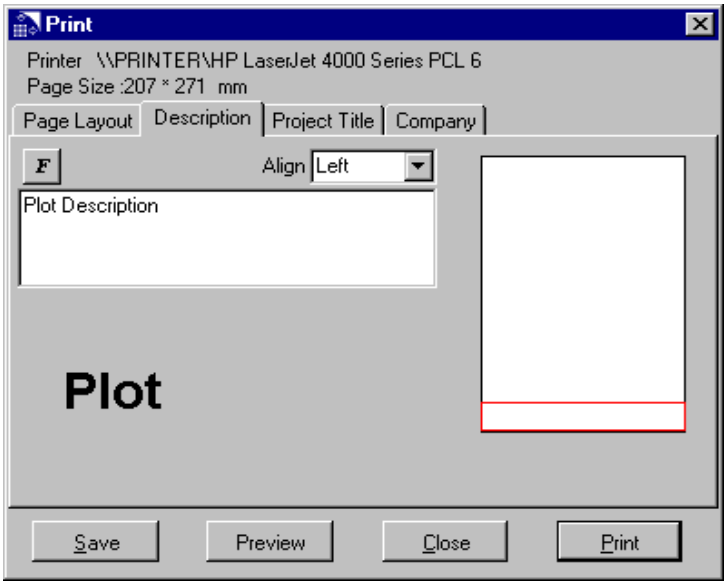
The Title blocks options are used to customize the appearance of the page layout as shown in the following figure (the actual arrangement and size of the title blocks on the page will vary depending on the number of title blocks selected). If the Plot Description, Project Title or Company Logo Title blocks are selected, an additional tab will be added to the Print window to accommodate these options.

- **Plot Borders** will plot an outline along the page margins
- **Plot description** will add a title block to display a description of the plot (see section Plot Description on page 325).
- Project Name will add a title block to display the Project Name and an optional bitmap image of a logo (see section Project Name on page 326).
- Company Name will add a title block to display the company name and an optional bitmap image of a logo (see section Company Name on page 327).
- Program Title will add a title block to display the Visual MODFLOW program information.



7.6.2 Plot Description

If the Description option is selected in the Page Layout tab, a Description tab will be active in the Print window as shown in the following figure.



To enter the Description of the plot simply click in the text box and start typing (or editing the current Description). A preview of the Description title block will appear in the space below the Description text box.

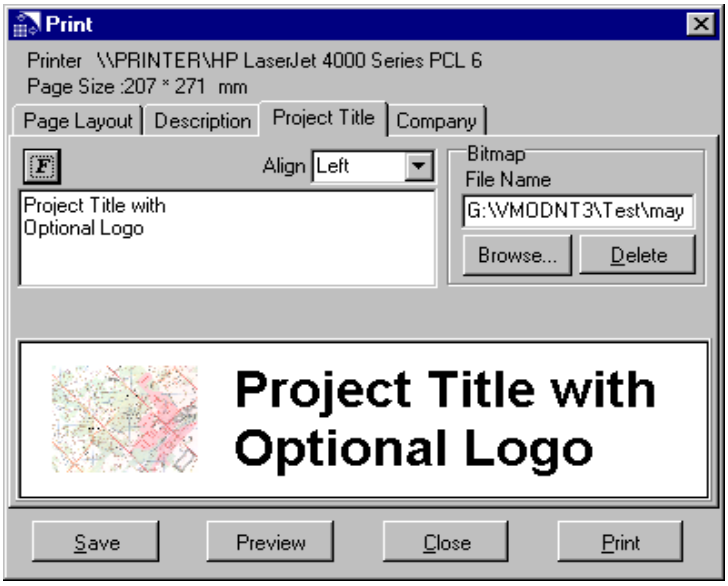
The font [***F***] button is used to select the desired font, size, style and color for the Description text.

The **Align** option is used to align the Description on the **Left**, **Center** or **Right** of the Description title block.

The Description information can be saved for subsequent printing of this information by clicking the [Save] button.

7.6.3 Project Name

If the Project Name option is selected in the Page Layout tab, a Project tab will be active in the Print window as shown in the following figure.



To enter the Project Name simply click in the text field and start typing (or editing the current Project Name).

The font [***F***] button is used to select the desired font, size, style and color for the Project Title text.

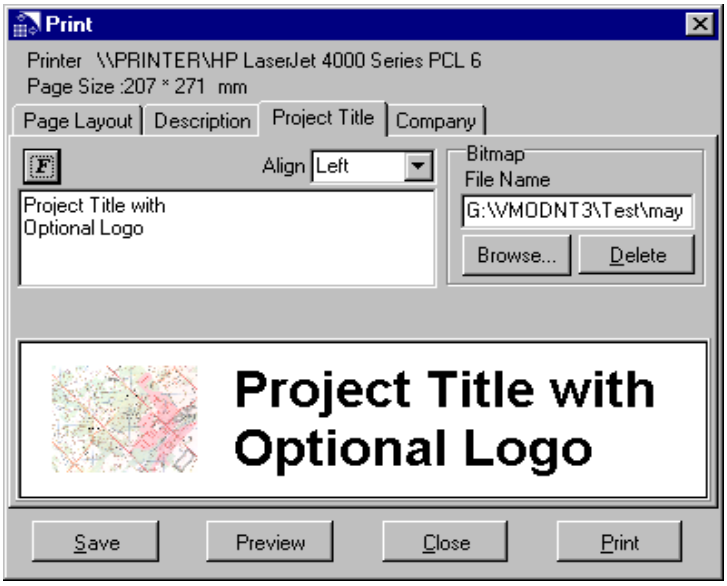
The **Align** option is used to align the Description on the **Left**, **Center** or **Right** of the Project Name title block.

The Bitmap option is used to import a bitmap image to display on the left of the Project Name title block. Use the [Browse] button to select the image file or use the [Delete] button to delete the selected image file.

The Project information can be saved for subsequent printing of this information by clicking the [Save] button.

7.6.4 Company Name

If the Company Name option is selected in the Page Layout tab, a Project Title tab will be activated in the Print window as shown in the following figure.



To enter the Company Name simply click in the text field and start typing (or editing the current Company Name).

The font [***F***] button is used to select the desired font, size, style and color for the Company Name text.

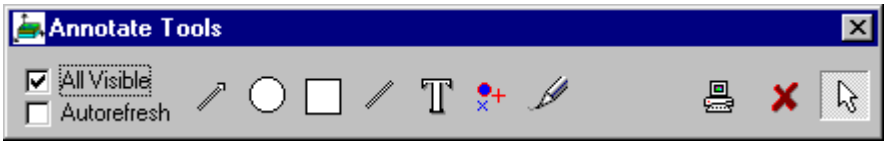
The **Align** option is used to align the Description on the **Left**, **Center** or **Right** of the Company Name title block.

The Bitmap option is used to import a bitmap image to display on the left of the Company Name title block. Use the [Browse] button to select the image file or use the [Delete] button to delete the selected image file.

The Company Name information can be saved for subsequent printing of this information by clicking the [Save] button.

7.6.5 Annotation Tools

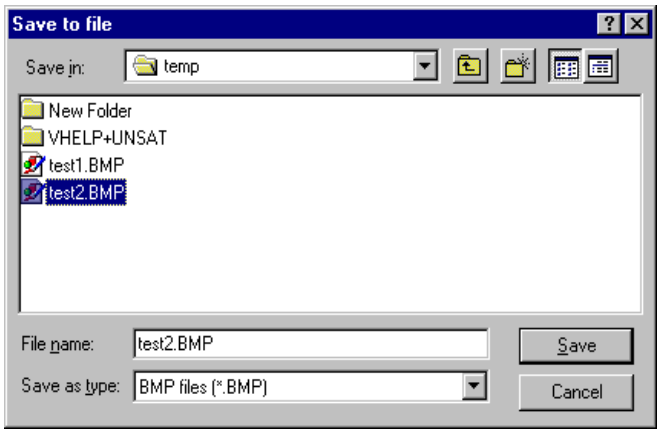
The image annotation options can be accessed by selecting **Edit/Annotation**. A floating **Annotation Tools** window will appear on the screen as shown in the following figure.



- Use the button to draw an arrow
- Use the button to draw a circle
- Use the button to draw a rectangle
- Use the button to draw a line
- Use the button to add text
- Use the button to add symbols
- Use the button to sketch a line
- Use the button to refresh the screen
- Use the button to delete a selected annotation object
- Use the button to select, re-size and move the annotation objects

7.6.6 Saving to a Graphics File

The image displayed in the **Image editor** window can also be saved to a graphics file by selecting **File/Save** as from the top menu bar. The following **Save to file** dialog will appear.



The 3D image can be saved to three different graphics formats:

- **Bitmap file (.BMP)**
- **Windows Metafile (.WMF)**
- **Enhanced Windows Metafile (.EMF)**

Either of these graphics files can be imported into most word processing software packages.

> **Note:** The resolution of the graphics file image will depend on your screen resolution and on the size of the **Image editor** window. In order to maximize the image quality you should maximize the **Image editor** window to full screen.

Alternatively, the image may be copied to the Windows clip board by selecting **Edit/ Copy to Clipboard** from the top menu bar, or clicking the **[Copy to Clipboard]** icon from the top toolbar. This image can be pasted into most word processing and graphics editing programs.

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A

Visual MODFLOW Data Files

Visual MODFLOW stores all of the data for the flow, pathline and contaminant transport model in a set of files having formats and data structures which are quite different than the model input data files required by MODFLOW, MODPATH, and MT3D. There are many reasons for these differences, but the primary reasons are:

- Visual MODFLOW does not require consistent units for length and time. Instead, Visual MODFLOW allows mixed units for different model parameters (e.g. length in metres, pumping rate in US GPM, Recharge rate in mm/yr)
- Visual MODFLOW does not require boundary conditions to be defined in terms of stress periods. Instead, Visual MODFLOW allows each boundary conditions to be defined in using real time values and raw field data.

These differences are two of the key elements that make Visual MODFLOW so practical and user-friendly. However, these differences also require Visual MODFLOW to store the data in a different format and then translate these data files to the required format prior to running the models.

The following sections lists the various input and output data files generated by Visual MODFLOW and describes the data format for some of the more important data files.

Most of input files are stored in ASCII text format, whereas most of the output files are stored in binary format. As a result, the input files can be manipulated using a text editor or even generated using a FORTRAN or Visual Basic program, rather than using Visual MODFLOW's graphical user interface. However, if the files are externally manipulated or generated, the useful data validation and formatting checks performed by Visual MODFLOW will not be available. As a result, special care must be taken so the data structure for these files is not corrupted. **It is not recommended - other than in special situations - to externally edit or manipulate the data files using a text editor.**

A.1Model Data Files

A.1.1 Visual MODFLOW Data Files

When a new data set is generated by Visual MODFLOW, a number of ASCII files are created. Each one of these data files must remain in the same directory to run Visual MODFLOW using this data set. These files are listed below, where *projectname* is the name assigned to the model. A description of the content of each file is given below.

The format of the files with an asterick (*) are detailed further in the next section.

General Files

projectname.*filename*.**DXF**	Imported AUTOCAD Data eXchange Format (DXF) drawing file
projectname.**MAP**	Map file created by Visual MODFLOW from a .DXF file
projectname.**EXT**	Visual MODFLOW file containing limits for DXF image
projectname.**INI**	Bitmap georeference data file
projectname.**LDB**	Temporary MSACCESS file for database control
projectname.**MDB**	Database file containing pumping well and observation well data
projectname.**MPS**	File containing general information for running MODPATH
projectname.**VMF**	General model setup and settings data file (XML format)
projectname.**VMN**	Annotation (lines, arrows, text, shapes) data file
projectname.**VMR**	Model run options data file

MODFLOW

projectname.**VIH**	Initial head data file
projectname.**VMB***	Flow Boundary condition data file
projectname.**VMG***	Grid discretization and geometry data file
projectname.**VMP***	Flow properties (Kx, Ky, Kz, Ss, Sy, Por, Recharge and Evapo-transpiration) data file
projectname.**VMO***	Head observation well data file
projectname.**VMO.GRP**	Head observation well groups data file
projectname.**VMW***	Pumping well data file

MODPATH

projectname.**VMA***	Particle location and tracking data file

MT3D

projectname.**MBT**	Basic transport data file

projectname.**MSS**	Source/sink data file
projectname.**MTD**	Dispersion data file
projectname.**MTH**	Recharge flux data file
projectname.**Conc001.MTI**	Initial concentration data for species 001
projectname.**MTN**	Constant concentration data file
projectname.**MTS**	Point source data file
projectname.**MTT**	Active/inactive transport cells data file
projectname.**MTH**	Evapotranspiration flux data file
*projectname***.VMT***	Concentration observation well data file
*projectname***.VMT.GRP**	Concentration observation well groups data file

Zone Budget

projectname.**VMZ**	Zone Budget zones data file

A.1.2 Numerical Model Input Files

The following files are generated by Visual MODFLOW during translation:

MODFLOW

MODFLOW**.IN**	List of translated files for MODFLOW
projectname.**BAS**	Basic Package data file
projectname.**BCF**	Block-Centred Flow Package data file.
projectname.**CHD**	Time-variant specified head data file
projectname.**DIS**	Model discretization data file
projectname.**DRN**	Drain Package data file
projectname.**EVT**	Evapotranspiration Package data file.
projectname.**GHB**	General-Head Boundary Package data file
projectname.**HFB**	Horizontal Flow Boundary Package data file.
projectname.**LPF**	Layer Property Flow data file
projectname.**OC**	Output control options data file
projectname.**PCG**	PCG2 Solver Package data file
projectname.**RCH**	Recharge Package data file
projectname.**RIV**	River Package data file
projectname.**SIP**	SIP Solver Package data file
projectname.**SOR**	SOR Solver Package data file
projectname.**STR**	Streamflow-Routing Package data file
projectname.**WEL**	Well Package data file
projectname.**WHS**	WHS Solver data file

MODPATH

BACKWARD.IN	Backward tracking particle locations data file
BACKWARD.PTH	Backward tracking run options data file
FORWARD.IN	Forward tracking particle locations data file
FORWARD.PTH	Forward tracking run options data file
projectname.**MPT**	Main MODPATH input data file
MODPATH.IN	List of MODPATH input files

MT3Dxx/RT3D

projectname.**AD3**	Advection data file
projectname.**BT3**	Basic Transport data file
projectname.**DP3**	Dispersion data file
projectname.**GCG**	Transport Solver data file
projectname.**RC3**	Chemical Reaction data file
projectname.**SS3**	Source / Sink Mixing data file
MT3D.IN	List if MT3D input files

Zone Budget

projectname.**ZBI**	Zone Budget data file
ZONEBUD.IN	List of Zone Budget input files

A.1.3 Output Files

After running the model, a number of results files will be generated. Some of the files generated by Visual MODFLOW can get very large (more than 100 Mbytes!). These files are typically in ASCII format, but some are in binary format to save disk space. The output files are described below.

Note

* The files marked with an asterisk can get quite large for transient simulations.

MODFLOW

projectname.**BGT***	MODFLOW file containing water budget data used by MODPATH (Binary format)
projectname.**DDN**	MODFLOW file containing drawdown X, Y, Z heads for each node (Binary format)
projectname.**DVT**	Visual MODFLOW file containing drawdown versus time results (Binary format)

projectname.**FLO***	MODFLOW file containing cell-by-cell flow terms (Binary format)
projectname.**HDS***	MODFLOW file containing head results (Binary format)
projectname.**LST***	MODFLOW listing file containing information and messages from (ASCII format)
projectname.**HVT**	Visual MODFLOW file containing head versus time results (Binary format)

MODPATH

projectname.**MPB**	MODPATH file containing backward tracking particle information (ASCII format)
projectname.**MPF**	MODPATH file containing forward particle information (ASCII format)
SUMMARY.PTH*	MODPATH file containing listing information and messages from MODPATH (ASCII format)

MT3Dxx/RT3D

projectname.**CNF***	MT3D file containing model grid configuration file (ASCII format)
projectname.**MAS***	MT3D file containing mass balance file (ASCII format)
projectname.**OBS***	MT3D file containing concentration at observation points (ASCII format)
projectname.**OT***	MT3D output file containing listing information and messages from MT3D (ASCII format)
projectname.**UCN***	MT3D file containing unformatted concentration information - (Binary format)

Zone Budget

projectname.**ZOT**	Zone Budget file containing water balance data (ASCII format)

A.2 Visual MODFLOW Input Data Formats

In the following sections, the formats of the Visual MODFLOW input data files are documented. This information is included for the experienced user only. It is not necessary to directly edit the data files. It is strongly recommended to always use the Visual MODFLOW graphical user interface to create and modify these files since this is the only way to assure the data files have the required format and valid data.

The information in the following formats is written from the bottom to the top. This is done to be consistent with MODFLOW. All input data files are written in free ASCII format, i.e., there is at least one blank space between the numbers in each line. Real numbers require a decimal point and can be expressed in either fixed or scientific

notation (e.g., 104.0 or 1.04E2). Integer numbers, however, **MUST NOT** contain a decimal point.

> **Note:** Spaces are the only delimiters accepted; commas are not accepted by Visual MODFLOW as delimiters.

VMA - Particle File Format

Particle data are stored as objects. Visual MODFLOW keeps on reading the objects until the end of the file is reached. The three types of particle objects are Single, Line and Circle particle objects.

For a Single particle object the format is:

0

1

Tracking *(0 = Backward , 1 = Forward)*

X Y Z Release_Time

For a Line particle object the format is:

1

N

Tracking *(0 = Backward , 1 = Forward)*

X_{START} Y_{START} Z_{START} Release_Time

X_{END} Y_{END} Z_{END} Release_Time

For a Circle particle object the format is:

2

N

Tracking *(0 = Backward , 1 = Forward)*

X_{CENTER} Y_{CENTER} Z_{CENTER} Release_Time

Radius

Plane *(0 = Along a layer, 1 = along a row, 2 = along a column)*

VMB - Flow Boundary Conditions File Format

Visual MODFLOW only saves boundary condition data for grid cells where boundary conditions are assigned.

The row, column, and layer indices in this file are slightly different than those displayed on the Reference cube and written to the MODFLOW files. In the .VMB file,

Rows are numbered from **0** to **NR-1**, beginning in the lower left-hand corner of the model (where NR is number of grid rows in the model)

Columns are numbered from **0** to **NC-1**, beginning in the lower left-hand corner of the model (where NC is number of grid columns in the model), and

Layers are numbered from **0** to **NL-1**, beginning at the bottom most layer of the model.

This contrasts with the MODFLOW files and the Reference cube, where cell (1,1,1) is located in the upper left corner of the top layer (when looking at the model in plan view on the screen).

The format of the data saved depends on the type of boundary condition in the grid cell. There are 5 boundary types in this file

0 Constant Head

1 River

2 General Head Boundary

3 Drain

4 Wall

Number_of_Layers

Number_of_Columns

Number_of_Rows

BLANK LINE

For each Constant Head boundary grid cell:

Layer

Column

Row

0 *(Code for Constant Head boundary type)*

Code_Number

Number_of_Time_Entries

$Start\_Time_1$ $Stop\_Time_1$ $Head_1$

.

$Start\_Time_{NE}$ $Stop\_time_{NE}$ $Head_{NE}$

For each River boundary grid cell:

Layer

Column

Row

1 *(Code for River Boundary type)*

Code_Number

Number_of_Time_Entries

$Start\_Time_1$ $Stop\_Time_1$ $River\_Stage_1$ $River\_Bottom_1$ $Conductance_1$

.

$Start\_Time_{NE}$ $Stop\_time_{NE}$ $River\_Stage_{NE}$ $River\_Bottom_{NE}$ $Conductance_{NE}$

For each General Head boundary grid cell:

Layer

Column

Row

2 *(Code for GHB Boundary type)*

Code_Number

Number_of_Time_Entries

$Start\_Time_1$ $Stop\_Time_1$ $General\_Head_1$ $Conductance_1$

.

$Start\_Time_{NE}$ $Stop\_time_{NE}$ $General\_Head_{NE}$ $Conductance_{NE}$

For each Drain Boundary grid cell:

Layer

Column

Row

3 *(Code for Drain Boundary type)*

Code_Number

Number_of_Time_Entries

$Start\_Time_1$ $Stop\_Time_1$ $Drain\_Elevation_1$ $Conductance_1$

.

$Start\_Time_{NE}$ $Stop\_time_{NE}$ $Drain\_Elevation_{NE}$ $Conductance_{NE}$

For each Wall boundary grid cell:

Layer

Column

Row

4 *(Code for Wall Boundary type)*

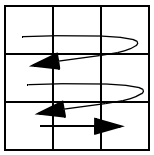
Face Conductivity Thickness

Parameter	Notes	Type
Face	1 = north, 2 = east, 3 = south, 4 = west	INTEGER

VMG - Grid File Format

The .VMG file contains the row and column coordinates, as well as the elevations of the top and bottom of each cell. It also contains a series of arrays to designate the active/inactive status of every cell.

Active Array

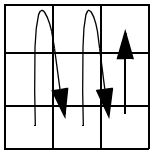


Looking down on the top of the model, the **active array** for each layer is written starting in the top left and ending in the bottom right

Each element = integer flag (1=active, 0=inactive)

Each line = one model row

Elevation Array



Looking down on the top of the model, the **elevation array** for each surface is written starting in the bottom left and ending in the top right

Each element = surface elevation

Each line = one model column

Number_of_columns

X_1

.

.

X_{NC+1} *(There is one more column line than the number of columns)*

Number_of_rows

Y_1

.

.

Y_{NR+1} *(There is one more row line than the number of rows)*

Number_of_layers

Z_1 *(Layer numbering starts at the bottom and goes to the top)*

.

.

.

Z_{NL+1} *(There is one more layer line than the number of layers)*

BLANK LINE

$Active\_array_{bottom\_layer}$

BLANK LINE

.

.

.

Active_array$_{top_layer}$

BLANK LINE

BLANK LINE

Number_of_columns

Number_of_rows

Number_of_layers

BLANK LINE

Elevation_array$_{bottom_surface}$

.

.

.

Elevation_array$_{top_surface}$

VMO - Heads Observation File Format

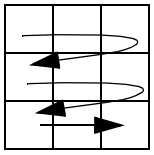
The .VMO and the .VMT files contain a two-line header followed by one entry for each head or concentration observation well.

Version='2.8.2.25'	*VMOD version number*
WellCount=32	*total number of observation wells in the file*
	for each observation well:
Well='obs 1'	w*ell name*
X= 403.2258065	x - *coordinate*
Y= 608.8709677	*y - coordinate*
Min_Z= 0	*bottom of model at observation location*
Max_Z= 25	*top of model at observation location*
Radius= 0	*well radius - not currently used*
ScreenCount=0	*not currently used for observation wells*
Screens	*not currently used for observation wells*
end Screens	*not currently used for observation wells*
ScheduleCount=0	*not currently used for observation wells*
Schedule	*not currently used for observation wells*
end Schedule	*not currently used for observation wells*
PointCount=1	*number of observation points in the well*

	for each observation point:
Point='Point #1'	*name of observation point*
Z= 12.5	*elevation of observation point*
SpeciesCount=1	*number of species in the model (for heads observation wells this is always 1)*
Species='Head'	*for head observation wells this value is always equal to "Head"; for concentration observation wells this is the species name*
ObsCount=1	*number of observation. times for this obs. point*
	for each observation time:
Time= 365	*observation time*
Value= 15	*head value*
end Species 'Head'	
end Point 'Point #1'	
end Well 'obs 1'	

VMP - Flow Property File Format

For each property (conductivity, storage, recharge, and evapotranspiration), the .VMP file contains a property value list followed by one integer array for each model layer. The integers in the arrays reference the property numbers in the property value list.



Looking down on the top of the model, the **Index array** for each layer is written starting in the top left and ending in the bottom right

Each element = integer flag = property index

Each line = one model row

Number_of_layers
Number_of_rows
Number_of_columns
Number_of_conductivity_properties (NK)
1 K_{X1} K_{Y1} K_{Z1}
...
NK K_{XNK} K_{YNK} K_{ZNK}
BLANK LINE
$Conductivity\_Index\_Array_{Bottom\_layer}$
BLANK LINE
...

Conductivity_Index_Array$_{Top_layer}$
BLANK LINE
Number_of_storage_properties (NS)
1 S_{S1} S_{Y1} Effective_porosity$_1$ Total_Porosity$_1$
...
NS S_{SNS} S_{YNS} Effective_Porosity$_{NS}$ Total_Porosity$_{NS}$
BLANK LINE
Storage_Index_Array$_{Bottom_layer}$
BLANK LINE
...
Storage_Index_Array$_{Top_layer}$
BLANK LINE
Number_of_recharge_properties (NR)
for each recharge property
Property_number Recharge_multiplier Index
Number_of_recharge_timesteps rchr entries
Property_number Recharge_value$_1$ Start_time$_1$ Stop_time$_1$
Property_number Recharge_value$_2$ Start_time$_2$ Stop_time$_2$
...
Property_number Recharge_value$_{nsteps}$ Start_time$_{nsteps}$ Stop_time$_{nsteps}$
BLANK LINE
Recharge_Index_Array$_{Bottom_layer}$
BLANK LINE
...
Recharge_Index_Array$_{Top_layer}$
BLANK LINE
Number_of_evapotranspiration_properties (NE)
for each evapotranspiration property
Property_number Evapo_multiplier Index
Number_of_evapo_timesteps evap entries
Property_number Evapo_value$_1$ Evapo_depth$_1$ Start_time$_1$ Stop_time$_1$
Property_number Evapo_value$_2$ Evapo_depth$_2$ Start_time$_2$ Stop_time$_2$
...
Property_number Evapo_value$_{nsteps}$ Evapo_depth$_{nsteps}$ Start_time$_{nsteps}$ Stop_time$_{nsteps}$
BLANK LINE
Evapo_Index_Array$_{Bottom_layer}$
BLANK LINE
...
Evapo_Index_Array$_{Top_layer}$

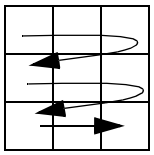
VMW - Pumping Well File Format

NW	Number_of_wells
	For each well (i = 1 to NW)
ActiveFlag	Active_flag *(1 = active, 0 = inactive)*
$WELL_i$, OBS_i	Name of pumping well and associated head observation well
X_i	X-coord
Y_i	Y-coord
$ZMIN_i$	Top elevation of model grid at (X, Y) location
$ZMAX_i$, R_i	Bottom elevation of model grid at (X, Y) location, Well Radius
NS_i	Number of well screen intervals
	For each screened interval (j = 1 to NS)
TOP_{ij}	Top elevation of Screen
BOT_{ij}	Bottom elevation of Screen
NT_i	Number of pumping time periods
	For each pumping time period (k = 1 to NT)
$START_{ik}$	Start time of time period
$STOP_{ik}$	Stop time of time period
$RATE_{ik}$	Pumping rate for time period

VMZ - Zone Budget File Format

The .VMZ file contains a cell-by-cell array for each layer with the zone number of each cell. The first array is for the bottom layer and the last array is for the top layer. Each cell can belong to only one user-specified zone.

Zone Index Array



Looking down on the top of the model, the **Zone Index array** for each layer is written starting in the top left and ending in the bottom right

Each element = integer zone number

Each line = one model row

Number_of_layers

Number_of_columns

Number_of_rows

Number_of_zones (Nzones)
1
2
...
Nzones
BLANK LINE
$Zone\_index\_array_{bottom}$
BLANK LINE
...
$Zone\_index\_array_{top}$

B

Interpolation Method Settings

Visual MODFLOW utilizes a built-in data interpolation, gridding and contouring component to import and interpolate field data. This component has been developed by Waterloo Hydrogeologic for the purpose of interpolating random data points to create a uniform grid of data for visualization and interpretation and utilization in Visual MODFLOW.

The interpolation methods currently supported by the Interpolation component include:

- Inverse Distance Squared,
- Natural Neighbor, and
- Kriging

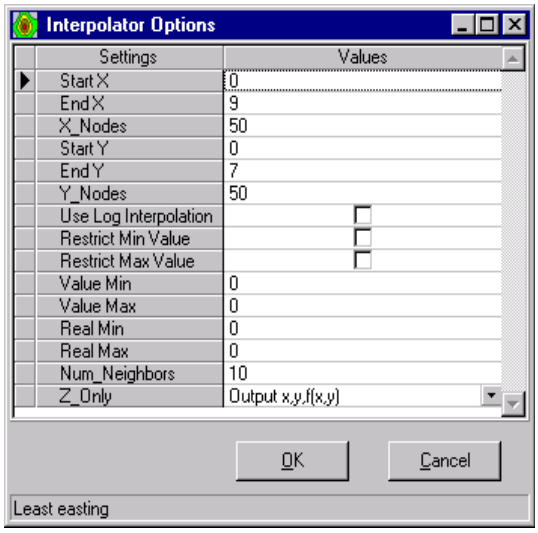
The following sections describe the methodology and the available settings for each of these interpolation methods. The method descriptions provided below are taken from GSLIB Geostatistical Software Library and User's Guide (Deutsch and Journel, 1998).

B.1 Inverse Distance Squared

The Inverse Distance Squared method is a very fast and efficient, weighted average interpolation method. The weighting factor applied to the data depends on the distance of the point from the grid cell and is inversely proportional to the distance squared. Consequently, the larger the distance of the data point is from the grid node, the smaller is the influence it has on the calculated value.

The Inverse Distance Squared method for interpolation may generate patterns similar to a "bull's-eye" surrounding points of observations. Selecting a larger number of nearest neighboring data points may smooth this effect, but if the bull's eye pattern is undesirable then other methods of interpolation like Natural Neighbour and Kriging are recommended.

The **Interpolator Options** window for the Inverse Distance Squared method is shown in the following figure while each of the settings parameters is described below.



Start X Minimum X co-ordinate for the interpolation grid.

End X Maximum X co-ordinate for the interpolation grid.

X_Nodes Number of grid nodes in the X-direction.

Start Y Minimum X co-ordinate for the interpolation grid.

End Y Maximum X co-ordinate for the interpolation grid.

Y-Nodes Number of grid nodes in the X-direction.

Use Log Interpolation Flag to interpolate the log values of the data.

Restrict Min Value Flag to restrict the minimum value of the interpolated data.

Restrict Max Value Flag to restrict the maximum value of the interpolation data.

Value Min Minimum value of the interpolated data. Any interpolated data less than **Value Min** will be assigned a value of **Value Min**.

Value Max Maximum value of the interpolated data. Any interpolated data greater than **Value Max** will be assigned a value of **Value Max**.

Real Min Real minimum value of interpolated data.

Real Max Real maximum value of interpolated data.

Num_Neighbors Number of nearest data points to use when calculating interpolated value for each grid node.

Z_Only

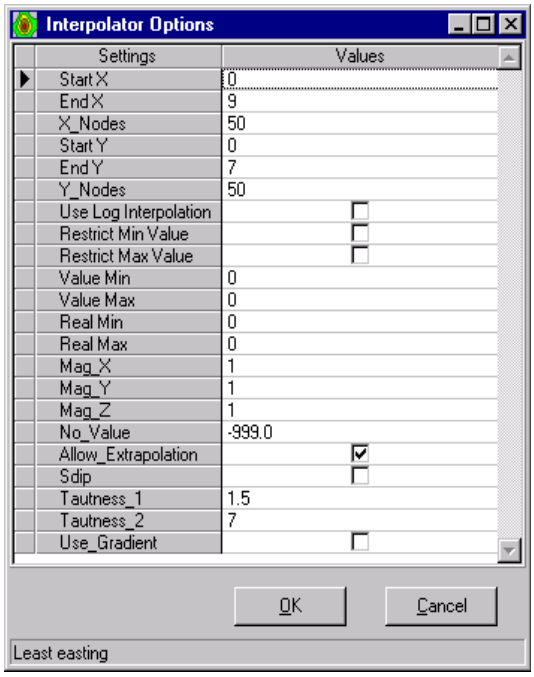
B.2 Natural Neighbor Method

The Natural Neighbor method (Watson, 1994) is based on the Thiessen polygon method used for interpolating rainfall data. The grid node for interpolation is considered a new point or target to the existing data set. With the addition of this point the Thiessen polygons based on the existing points are modified to include the new point. The polygons reduce in area to include the new points and the area that is taken out from the existing polygons is called the “borrowed area”. The interpolation algorithm calculates the interpolated value as the weighted average of the neighboring observations where the weights are proportional to the borrowed areas. The Natural neighbor method is valid only with the convex hull of the Thiessen polygon formed by the data points and values outside the hull extrapolation should be used with caution.

The natural neighbor interpolation scheme may be visualized as a taut rubber sheet stretched to satisfy all the data points. The interpolated value at any location is a linear combination of all natural neighbors of that location, and the resulting surface is continuous with a slope that is also continuous. Combining the gradients or slopes with the linear interpolation provides results that is more smooth and may anticipate the peaks and valleys between data. Singularities and other undesirable effects may be lessened by incorporating the gradient factor.

The gradient influence on the results can be manipulated by two tautness parameters that the user can enter. These parameters allow the interpolated surface to vary from purely linear interpolation to one which is well rounded and has the gradient factor. In all cases the slope discontinuities are removed and the resulting surface has slope continuity everywhere.

The **Interpolator Options** window for the Natural Neighbor method is shown in the following figure while each of the settings parameters is described below.



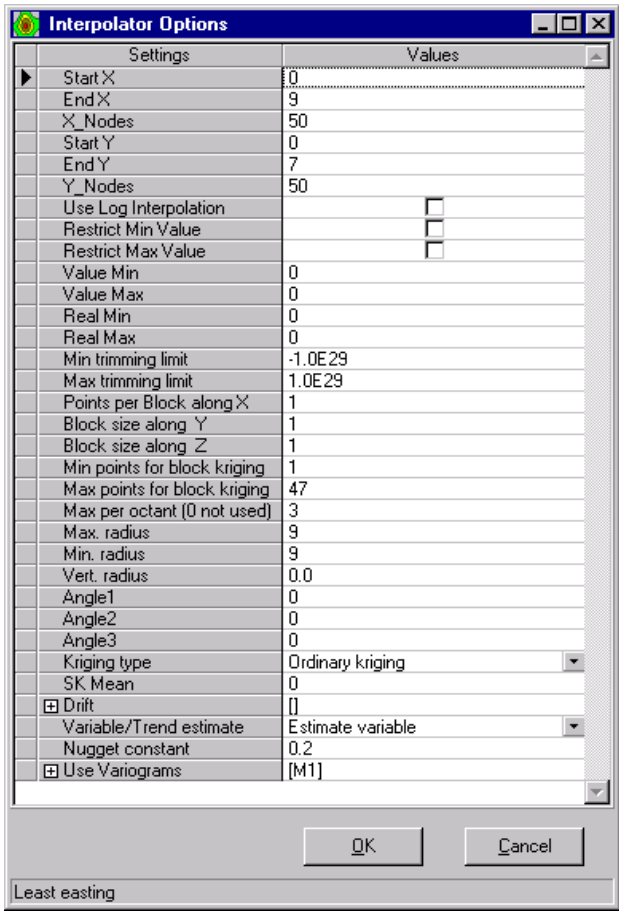
Start X	Minimum X co-ordinate for the interpolation grid.
End X	Maximum X co-ordinate for the interpolation grid.
X_Nodes	Number of grid nodes in the X-direction.
Start Y	Minimum X co-ordinate for the interpolation grid.
End Y	Maximum X co-ordinate for the interpolation grid.
Y-Nodes	Number of grid nodes in the X-direction.
Use Log Interpolation	Flag to interpolate the log values of the data.
Restrict Min Value	Flag to restrict the minimum value of the interpolated data.
Restrict Max Value	Flag to restrict the maximum value of the interpolation data.
Value Min	Minimum value of the interpolated data. Any interpolated data less than **Value Min** will be assigned a value of **Value Min**.
Value Max	Maximum value of the interpolated data. Any interpolated data greater than **Value Max** will be assigned a value of **Value Max**.
Real Min	Real minimum value of interpolated data.
Real Max	Real maximum value of interpolated data.
Mag_X	X-co-ordinate magnification factor
Mag_Y	Y-co-ordinate magnification factor
Mag_Z	Z-co-ordinate magnification factor

No_Value	Value assigned to nodes located outside the convex hull of the data points (where interpolation is not performed)
Allow_Extrapolation	Is a flag to use extrapolation for nodes outside the convex hull of the polygon formed by the data points. In this case linear regression is used to fit a plane through the data set and calculate the interpolated value. This should be used with caution since extrapolation is less reliable than interpolation.
Sdip	Calculate the aspect and slope at each grid node and this can be used to augment the elevation information. The aspect is measured in degrees or radians clockwise from north and the slope is measured positively below the horizontal plane in degrees or radians.
Tautness_1	Controls the influence of the gradient on the results and may be used to smooth the interpolated surface.
Tautness_2	Controls the influence of the gradient on the results and may be used to smooth the interpolated surface.
Use_Gradient	Blends the gradient calculation and the linear interpolation calculation to produce a smoother surface.

B.3 Kriging

Kriging is a geostatistical method that produces visually appealing maps from irregularly spaced data. Anisotropy and underlying trends suggested in the data can be incorporated in an efficient manner through kriging. The program used called kt3d is available in the public domain from the Geostatistical Software Library (GSLIB) distributed by Stanford University and is well-documented by Deustch and Journel (1998). The program kt3d from GSLIB performs simple kriging, ordinary kriging, or kriging with a polynomial trend and uses the standard parameter file used by GSLIB. If the semi-variogram components have already been modeled by the user they can be incorporated into the program by choosing the appropriate set of parameters in the parameter file. The semi-variograms available include Spherical, Exponential, Gaussian, Power and the Hole effect models. If the variogram information is not available, the default linear variogram with no nugget effect should be used. This option is a special case of the Power model with the exponent equal to 1.

The **Interpolator Options** window for the Natural Neighbor method is shown in the following figure while each of the settings parameters is described below.



Start X	Minimum X co-ordinate for the interpolation grid.
End X	Maximum X co-ordinate for the interpolation grid.
X_Nodes	Number of grid nodes in the X-direction.
Start Y	Minimum X co-ordinate for the interpolation grid.
End Y	Maximum X co-ordinate for the interpolation grid.
Y-Nodes	Number of grid nodes in the X-direction.
Use Log Interpolation	Flag to interpolate the log values of the data.
Restrict Min Value	Flag to restrict the minimum value of the interpolated data.
Restrict Max Value	Flag to restrict the maximum value of the interpolation data.
Value Min	Minimum value of the interpolated data. Any interpolated data less than **Value Min** will be assigned a value of **Value Min**.
Value Max	Maximum value of the interpolated data. Any interpolated data greater than **Value Max** will be assigned a value of **Value Max**.

Real Min	Real minimum value of interpolated data.
Real Max	Real maximum value of interpolated data.
Min Trimming Limit	Minimum bound for the interpolated data if the **Restrict Min Value** option is not selected by the user.
Max Trimming Limit	Maximum bound for the interpolated data if the **Restrict Max Value** option is not selected by the user.

The **Points per block along X**, **Points per block along Y** and **Points per block along Z** values allow the user to choose Block Kriging used for interpolation as compared to Point Kriging. Block Kriging is based on the premise that since Kriging is a linear algorithm, and direct estimation of the block average is possible for user-defined blocks. The default values for these parameters are 1 and in this case the default method is Point Kriging. If Block Kriging is being used, the user needs to enter the **Min points for block kriging** and **Max points for block kriging**.

The Octant Search option is an exhaustive search option available to make sure that data are taken on all sides of the point being estimated and is especially recommended for 3D data. If the user specifies **Max points per octant** to be greater than 0, an Octant Search is employed to find the neighborhood of points for interpolation.

The **Max radius** and **Min radius** defines the search distances in user specified units in the maximum horizontal direction and the minimum horizontal direction for determining the neighborhood of points for interpolation. For isotropic data the two radii are the same. Enter the **Vertical Radius** value if 3D Kriging is to be performed. If the total number of points in the data is large (>200) computation time for Kriging may be reduced by specifying a smaller radius for the search.

The **Angle1**, **Angle2** and **Angle3** parameters define the search ellipsoid for situations in which anisotropy is present in the data.

The **Kriging type** options are

- **Stationary simple Kriging with SK mean**
- **Ordinary kriging**
- **Nonstationary simple Kriging with means from an external file**
- **Kriging with external drift**

The following guidelines are recommended for selecting the type of Kriging.

Choose **Stationary simple Kriging with SK mean**, if the mean value is known and is constant throughout the area.

Select **Ordinary Kriging** if the mean is not constant everywhere, and needs to be recalculated dependent on the location of the neighborhood.

Choose **Nonstationary simple kriging with means from an external file** if the mean is not constant and has to be read from an external file.

Select **Kriging with an external drift** when only the trend component needs to be estimated and not the residual component, where the variable is assumed to be the sum

of the trend and the residual component. This option is also referred to as Universal Kriging.

For most situations **Ordinary Kriging** is recommended and is the default option.

The **SK Mean** defines the global mean of the data if **Stationary simple Kriging** is performed.

The **Drift** term defines the drift components if **Kriging with external drift** is performed. Nine drift components are possible:

- X = linear drift in x
- Y = linear drift in y
- Z = linear drift in z
- Xq = quadratic drift in x
- Yq = quadratic drift in y
- Zq = quadratic drift in z
- XY = cross quadratic drift in xy
- XZ = cross quadratic drift in xz
- YZ = cross quadratic drift in yz

The **Variable/Trend Estimate** allows the user to choose between estimating the variable or the trend. The default is **Estimate variable**.

The **Nugget** constant quantifies the sampling and assaying errors in the data. In a Variogram plot the nugget constant is the y-intercept value.

The **Use variograms** option allows the user to select the type of variogram to be used. The Variogram models available include:

- **Spherical**
- **Exponential**
- **Gaussian**
- **PowerHole Effect**

If the variogram information is not available, the default linear variogram with no nugget effect should be used. This option is a special case of the **Power** model with the exponent equal to 1.

C

Numeric Engines

Visual MODFLOW supports all of the most recent public domain and proprietary versions of MODFLOW and MT3D for simulating groundwater flow modeling and mass transport modeling, respectively. In Visual MODFLOW, these programs are referred to as Numeric Engines because they perform the numeric calculations required to solve the finite difference equations of groundwater flow and mass transport. The numeric engines supported by Visual MODFLOW include:

Groundwater Flow

- MODFLOW-96 (Public Domain, U.S. Geological Survey)
- MODFLOW-2000 (Public Domain, U.S. Geological Survey)

Mass Transport

- MT3Dv1.5 (Public Domain, U.S. Dept. of Defence)
- MT3D96 (Proprietary, S.S. Papadopulos & Associates, Inc.)
- MT3DMS (Public Domain, U.S. Army Corp of Engineers)
- MT3D99 (Proprietary, S.S. Papadopulos & Associates, Inc.)
- RT3Dv1.0 (Public Domain, Battelle Northwest Laboratories)
- RT3Dv2.5 (Public Domain, Battelle Northwest Laboratories)

Although the most recent versions of these programs are going to be used the majority of the time, the reason for continuing to support the legacy codes is to give the user the opportunity to reproduce simulation results from older model data sets using exactly the same simulation programs.

> **Note:** The MODPATH and Zone Budget versions included in Visual MODFLOW are the latest U.S.Geological Survey versions, compiled and optimized to run as 32 bit native Windows applications.

The following sections provide a brief overview of each Flow and Transport Numeric Engine and offer some insight into the differences between them.

C.1 Groundwater Flow Numeric Engines

MODFLOW is a MODular finite-difference ground-water FLOW model originally developed by the U.S. Geological Survey and released to the public domain in 1983. This version was referred to as MODFLOW-83. This code was eventually updated to conform to the Fortran 77 programming language in McDonald and Harbaugh (1988). The revised program was referred to as MODFLOW-88 and was also released to the public domain.

Included with your Visual MODFLOW Installation CD-ROM is a document file of the original MODFLOW-88 Reference Manual (**MODFLOW-88 Manual.pdf**) and it can be found in the **Manuals** directory on the Installation CD.

MODFLOW-96

MODFLOW-96 was released by the U.S. Geological Survey in 1996 to address several perceived needs of the program, most notably the ability to converted dry cells to variable head cells, and the ability to calculate alternate interblock transmissivities.

Included with your Visual MODFLOW Installation CD-ROM is a document file of the original MODFLOW-96 Reference Manual (**MODFLOW-96 Manual.pdf**) and it can be found in the **Manuals** directory on the Installation CD.

MODFLOW-2000

MODFLOW-2000 was released by the U.S. Geologic Survey in 2000 and introduced a new process-based approach to the MODFLOW program structure, together with built-in parameter estimation capabilities. The process-based approach and built-in parameter estimation required some radical changes to input file structures and data requirements, the most significant being:

- The Block-Centered Flow (BCF) Package was replaced by the Layer Property Flow (LPF) Package
- The top and bottom elevation of each grid cell must be explicitly defined
- The boundary conditions values and property values may be defined in terms of parameter values and multiplier arrays.

Visual MODFLOW supports and includes both MODFLOW-96 and MODFLOW-2000 to run the groundwater flow simulation. Ideally, these programs should produce identical results. However, MODFLOW-2000 may produce some subtle differences when running MODFLOW-96 models if specified VCONT values were used to simulate leakage from an aquitard.

Included with your Visual MODFLOW Installation CD-ROM is a document file of the original MODFLOW-2000 Reference Manual (**MODFLOW-2000 Manual.pdf**) and it can be found in the **Manuals** directory on the Installation CD.

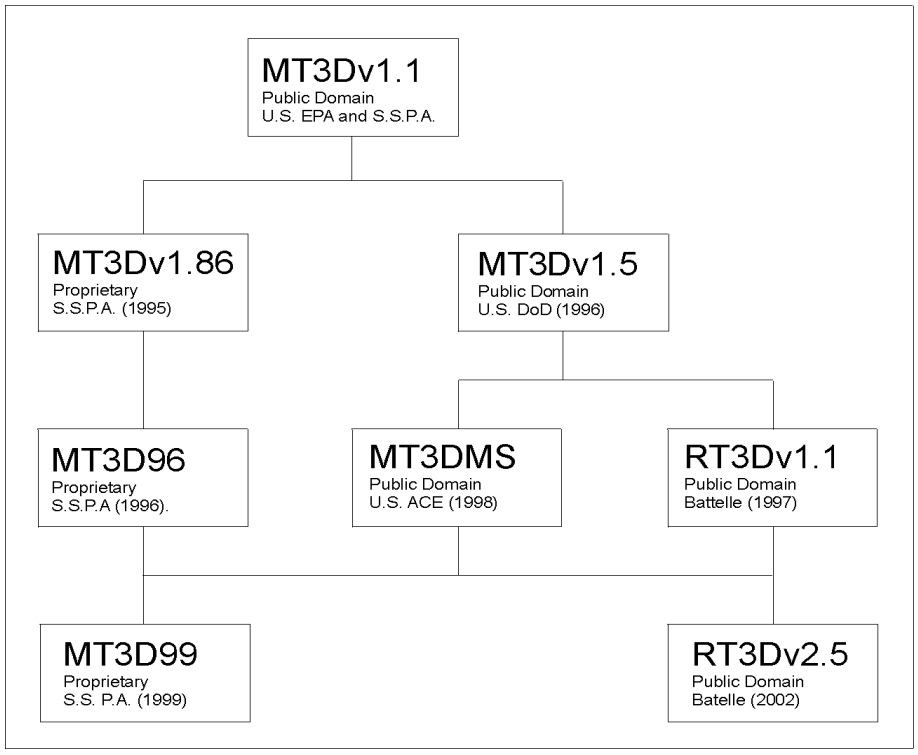
C.2 Mass Transport Numeric Engines

All of the different mass transport programs supported by Visual MODFLOW have evolved from essentially the same version of MT3D (Mass Transport in 3 Dimensions) first developed by Chunmiao Zheng in 1990 at S.S. Papadopulos & Associates, Inc. with partial support from the U.S. Environmental Protection Agency (USEPA).

MT3D uses either a mixed Eulerian-Lagrangian approach or the finite-difference method to solve the three-dimensional advective-dispersive-reactive equation. It is based on a modular structure to permit simulation of transport components independently or jointly. MT3D interfaces directly with the U.S. Geological Survey finite-difference groundwater flow model, MODFLOW, for the head solution, and supports most hydrologic and discretization features of MODFLOW.

MT3D was released as a public domain code in 1990 and since then has been widely accepted by practitioners and researchers around the world. Since the first release there have been several new proprietary and public domain versions of MT3D developed to enhance the analysis features, fix defects and provide better numerical efficiency.

The following flowchart illustrates the evolution of the MT3D transport engines.



The differences between the various Transport Numeric Engines are primarily rooted in the options for specifying options for sorption, reactions and solvers as summarized in the following table.

		MT3D150	MT3D96	RT3Dv1.0	MT3DMS	MT3D99	RT3Dv2.5
Sorption Options	No Sorption is simulated	✓	✓	✓	✓	✓	✓
	Linear Isotherm (equilibrium-controlled)	✓	✓	✓	✓	✓	✓
	Freundlich Isotherm (equilibrium-controlled)	✓	✓	✓	✓	✓	✓
	Langmuir Isotherm (equilibrium-controlled)	✓	✓	✓	✓	✓	✓
	First-order kinetic sorption (non-equilibrium)				✓	✓	
	First-order kinetic dual-domain mass transfer				✓	✓	
Reactions Options	No kinetic reaction	✓	✓	✓	✓	✓	✓
	First-order irreversible decay	✓	✓		✓	✓	✓
	Monod kinetics					✓	
	First-order parent-daughter chain reaction					✓	
	Instantaneous reactions among species					✓	
	Instantaneous aerobic decay of BTEX			✓			✓
	Instantaneous multi-path degradation of BTEX			✓			✓
	Kinetic limited multi-path degradation of BTEX			✓			✓
	Rate-limited sorption reactions			✓			✓
	Double-Monod degradation model			✓			✓
	Sequential decay reactions			✓			✓
	Aerobic/anaerobic model for PCE/TCE degrad.			✓			✓
Solver	MOC, MMOC, HMOC and Upstream FD	✓	✓	✓	✓	✓	✓
	Total-Variation Diminishing (TVD)				✓	✓	✓
	Generalized Conjugate Gradient (GCG)				✓	✓	✓

MT3Dv1.5

MT3D is a modular three-dimensional transport model for simulation of advection, dispersion and chemical reaction of contaminants in groundwater systems. C. Zheng developed this transport model in 1996 while working at S.S. Papadopulos. The U.S. Environmental Protection Agency paid for the development of the documentation and, in return, a limited public domain version was made available. C. Zheng further developed MT3D at the University of Alabama with a grant from the Department of Defense.

Included with your Visual MODFLOW Installation CD-ROM is a document file of the original MT3D 1.1 Reference Manual. This is also the manual for MT3Dv1.5. The name of this file is **MT3D1.1 manual.pdf** and it can be found in the **Manuals** directory on the Installation CD.

MT3D ^{96}

C. Zheng developed this upgrade to the MT3D 1.5 code in 1996 for S.S. Papadopulos & Associates, Inc. The major modifications and enhancements from MT3D 1.5 include:

- improved Eulerian-Lagrangian solutions
- improved finite-difference solution
- improved treatment of heterogeneous porosity and transient flow problems
- expanded mass accounting
- more flexible input for chemical reactions
- time-varying constant-concentration boundary conditions
- improved interface with MODFLOW
- full backward compatibility with previous versions of MT3D

At the time of it's release, MT3D96 was a proprietary program sold by S.S. Papadopulos & Associates, Inc.and was not available in the public domain. The MT3D96 program was replaced by MT3D99 and is now considered to be obsolete.

However, Visual MODFLOW continues to support MT3D96 to ensure historical modeling results may be reproduced using exactly the same simulation codes. MT3D96 may be purchased as an add-on package to Visual MODFLOW.

MT3D MS

MT3DMS is a modular three-dimensional multi-species transport model for simulation of advection, dispersion and chemical reactions of contaminants in groundwater systems. C. Zheng and P.P. Wang developed this multi-species transport model in June 1998 for the US Army Corps of Engineers. This model includes the addition of:

- a third-order total-variation-diminishing scheme for solving the advection term, an iterative solver based on generalized conjugate gradient methods and the Lanczos/ORTHOMIN acceleration scheme,

- options for accommodating non-equilibrium sorption and dual-domain advection-diffusion mass transport, and
- a multi-component program structure to accommodate add-on reaction packages.

Included with your Visual MODFLOW Installation CD-ROM is a document file of the MT3DMS Reference Manual. The name of this file is **MT3DMS manual.pdf** and it can be found in the **Manuals** directory of the Installation CD. Please refer to this document for a detailed description of both the sorption options, reaction packages and solvers available.

MT3D 99

MT3D99 is an upgrade to MT3D96 and incorporates many of the same functions as MT3DMS together with some additional modifications and enhancements including:

- zero-order and mixed-order Monod kinetic reactions;
- a reaction package to handle BIOPLUME-type aerobic and anaerobic reactions between hydrocarbon contaminants and any user-specified electron acceptors and parent-daughter chain reactions for inorganic and organic compounds;
- automatic restart option; and
- detailed cell-by-cell mass budgets.

MT3D99 is a proprietary program developed by C.Zheng under contract to S.S. Papadopulos & Associates, Inc. and must be purchased as an add-on package to Visual MODFLOW.

Included with your Visual MODFLOW Installation CD-ROM is a document file of the MT3D99 Reference Manual. Please refer to this manual for a detailed description of both the sorption options, reaction packages and solvers available.

RT3D

RT3D is a program for simulating reactive multi-species mass transport in three-dimensional groundwater aquifers. RT3Dv1.0 was first developed by P.T. Clement in 1997 for the Battelle Memorial Institute, Pacific Northwest National Laboratory and was subsequently released into the public domain and quickly became an accepted standard for reactive transport modeling. Unfortunately, the code was based on MT3Dv1.5 and did not include many of the new solver technology implemented in MT3DMS. As a result, the application of RT3D was always crippled by excessively slow run-times.

RT3Dv2.5 was released to the public domain in 2002 and now includes the same solver options as MT3DMS.

Included with your Visual MODFLOW Installation CD-ROM is a document file of the original RT3D Reference Manual (**RT3D V1.0 manual.pdf**) together with the RT3D

v2.5 Update Document (**RT3D V2.5 Update.pdf**). These files can be found in the **Manuals** directory of the Installation CD.

The RT3D Transport Numeric Engine contains the following reaction packages:

- Instantaneous aerobic decay of BTEX
- Instantaneous multi-path degradation of BTEX
- Kinetic limited multi-path degradation of BTEX
- Rate-limited sorption reactions
- Double-Monod degradation model
- Sequential decay reactions
- Aerobic/anaerobic model for PCE/TCE degradation

The following sections, taken from the RT3D Manual, briefly outline each of the reaction packages. For more information on appropriate values for the reaction constants, please see the RT3D Reference Manual.

For each RT3D reaction model, it is the user's responsibility obtain a detailed understanding of the limitations of the reaction model by refering to the RT3D Reference Manual and obtaining copies of the referenced research papers before using the model for professional purposes.

Note: Stoichiometric ratios and yield coefficients in RT3D are assumed to be mass-based rather than molar based. Concentrations in Visual MODFLOW for RT3D based models are in the concentration units specified by the user.

Model 1 - Instantaneous Aerobic Decay of BTEX

Model 1 simulates the instantaneous biodegradation of fuel hydrocarbons under aerobic conditions. At each time step, the reaction algorithm models removal rates by reducing either hydrocarbons or oxygen to zero within each grid cell.

Model 1 has two components, BTEX and Oxygen, both of which are mobile and one reaction constant, the Stoichiometric ratio of Oxygen to BTEX (Default = 3.14).

Model 2 - Instantaneous Degradation of BTEX using Multiple Electron Acceptors

Model 2 is similar to the previous package except that it uses five degradation pathways (aerobic respiration, denitrification, iron reduction, sulfate reduction, and methanogenesis) to simulate biodegradation of BTEX compounds.

Model 2 includes six mobile components, BTEX, Oxygen, Nitrate, Fe2+, Sulfate, and Methane and the following reaction constants:

- RC1, Max. concentration of Fe2+ (default = 0 mg/L or 0 ug/L)
- RC2, Max. concentration of Methane (default = 0 mg/L or 0 ug/L)
- RC3, Stoichiometric ratio of Oxygen (consumed) to BTEX (default = 3.14)

- RC4, Stoichiometric ratio of Nitrate (consumed) to BTEX (default = 4.9)
- RC5, Stoichiometric ratio of Fe2+ (produced) to BTEX (default = 21.8)
- RC6, Stoichiometric ratio of Sulfate (consumed) to BTEX (default = 4.7)
- RC7, Stoichiometric ratio of Methane (produced) to BTEX (default = 0.78)

Model 3 - Kinetic-limited Degradation of BTEX using Multiple Electron Acceptors

Model 3 is similar to Model 2, however, it uses kinetic-limited reactions rather than instantaneous reactions. The model predicts a rate of hydrocarbon decay that is proportional to species concentrations. Monod-type kinetics are used to account for electron acceptor concentrations and an inhibition model is used to simulate the sequential electron acceptor utilization process.

This package uses six mobile components: BTEX, Oxygen, Nitrate, Fe2+, Sulfate, and Methane. This package uses the following reaction constants:

- RC1, Max. concentration of Fe2+ (default = 0 mg/L or 0 ug/L)
- RC2, Max. concentration of Methane (default = 0 mg/L or 0 ug/L)
- RC3, Hydrocarbon decay rate via aerobic process (default = 0 T^{-1})
- RC4, Hydrocarbon decay rate via denitrification (default = 0 T^{-1})
- RC5, Hydrocarbon decay rate via iron reduction (default = 0 T^{-1})
- RC6, Hydrocarbon decay rate via sulfate reduction (default = 0 T^{-1})
- RC7, Hydrocarbon decay rate via methanogenesis (default = 0 T^{-1})
- RC8, Half saturation constant for Oxygen (default = 0.5 mg/L or 500 ug/L)
- RC9, Half saturation constant for Nitrate (default = 0.5 mg/L or 500 ug/L)
- RC10, Half saturation constant for Fe3+ (default = 0.5 mg/L or 500 ug/L)
- RC11, Half saturation constant for Sulfate (default = 0.5 mg/L or 500 ug/L)
- RC12, Half saturation constant for Methane (default = 0.5 mg/L or 500 ug/L)
- RC13, Inhibition coefficient for Oxygen reaction (default = 0.01 mg/L or 10 ug/L)
- RC14, Inhibition coefficient for Nitrate reaction (default = 0.01 mg/L or 10 ug/L)
- RC15, Inhibition coefficient for Fe3+ reaction (default = 10 mg/L or 10000 ug/L)
- RC16, Inhibition coefficient for Sulfate reaction (default = 0.01 mg/L or 10 ug/L)
- RC17, Oxygen yield coefficient (default = 3.14)
- RC18, Nitrate yield coefficient (default = 4.9)
- RC19, Fe2+ production yield coefficient (default = 21.8)
- RC20, Sulfate yield coefficient (default = 4.7)
- RC21, Methane production yield coefficient (default = 0.78)

Model 4 - Rate Limited Sorption Reactions

Model 4 simulates mass-transfer-limited sorption reactions and tracks one mobile and one immobile fraction of the same species. The mobile component, *Aqueous_conc*, and the immobile component, *Solid_conc*. Only two reaction parameters are need; the mass transfer coefficient and the linear partitioning coefficient. Note that the linear partitioning coefficient is effectively the same as a distribution coefficient, Kd.

Model 5 - Double Monod Model

Model 5 simulates electron donor and acceptor reactions mediated by bacterial growth in the aqueous and soil phase. Because this model describes a general double Monod model, it can be used to model any type of biological system, provided that accurate yield coefficients and rate constants are available.

Model 5 includes three mobile and one immobile components (*eDonor*, *eAcceptor*, *Aqu. Bact.*, and *Soil Bact)* and eight reaction constants.

- RC1, Specific utilization rate (default = 0 T^{-1})
- RC2, Monod half saturation constant for eDonor (default = 0 mg/L or 0 ug/L)
- RC3, Monod half saturation constant for eAcceptor (default = 0 mg/L or 0 ug/L)
- RC4, Biomass produced per unit amount of electron donor utilized (default = 0)
- RC5, Electron acceptor used per unit amount of electron donor utilized (default = 0)
- RC6, First-order bacterial decay rate (default = 0 T^{-1})
- RC7, First-order bacterial attachment rate (default = 0 T^{-1})
- RC8, First-order bacterial detachment rate (default = 0.5 T^{-1})

Model 6 - Sequential Decay Reactions

Model 6 simulates sequential degradation of up to four components using a series of parent-daughter reactions under anaerobic conditions.

By default, Model 6 has been set up for modeling the dechlorination of PCE, but in principle any four-species sequential decay reaction could be specified. Thus, Model 6 has four mobile components: PCE, TCE, DCE, and VC. It has seven reaction constants.

- RC1, PCE first-order degradation rate (default = 0 T^{-1})
- RC2, TCE first-order degradation rate (default = 0 T^{-1})
- RC3, DCE first-order degradation rate (default = 0 T^{-1})
- RC4, VC first-order degradation rate (default = 0 T^{-1})
- RC5, TCE to PCE yield coefficient (default = 0.792)
- RC6, DCE to TCE yield coefficient (default = 0.738)
- RC7, VC to DCE yield coefficient (default = 0.644)

Model 7 - Aerobic/Anaerobic Model for PCE/TCE Degradation

Model 7 simulates both aerobic and anaerobic degradation of chlorinated solvents. It includes six mobile components (PCE, TCE, DCE, VC, ETH, and Cl) and nine reaction constants.

- RC1, Anaerobic reaction rate for PCE (default = 0 T^{-1})
- RC2, Anaerobic reaction rate for TCE (default = 0 T^{-1})
- RC3, Aerobic decay rate for TCE (default = 0 T^{-1})
- RC4, Anaerobic reaction rate for DCE (default = 0 T^{-1})
- RC5, Aerobic decay rate for DCE (default = 0 T^{-1})

- RC6, Anaerobic reaction rate for VC (default = 0 T^{-1})
- RC7, Aerobic decay rate for VC (default = 0 T^{-1})
- RC8, Anaerobic reaction rate for ETH (default = 0 T^{-1})
- RC9, Aerobic decay rate for ETH (default = 0 T^{-1})

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